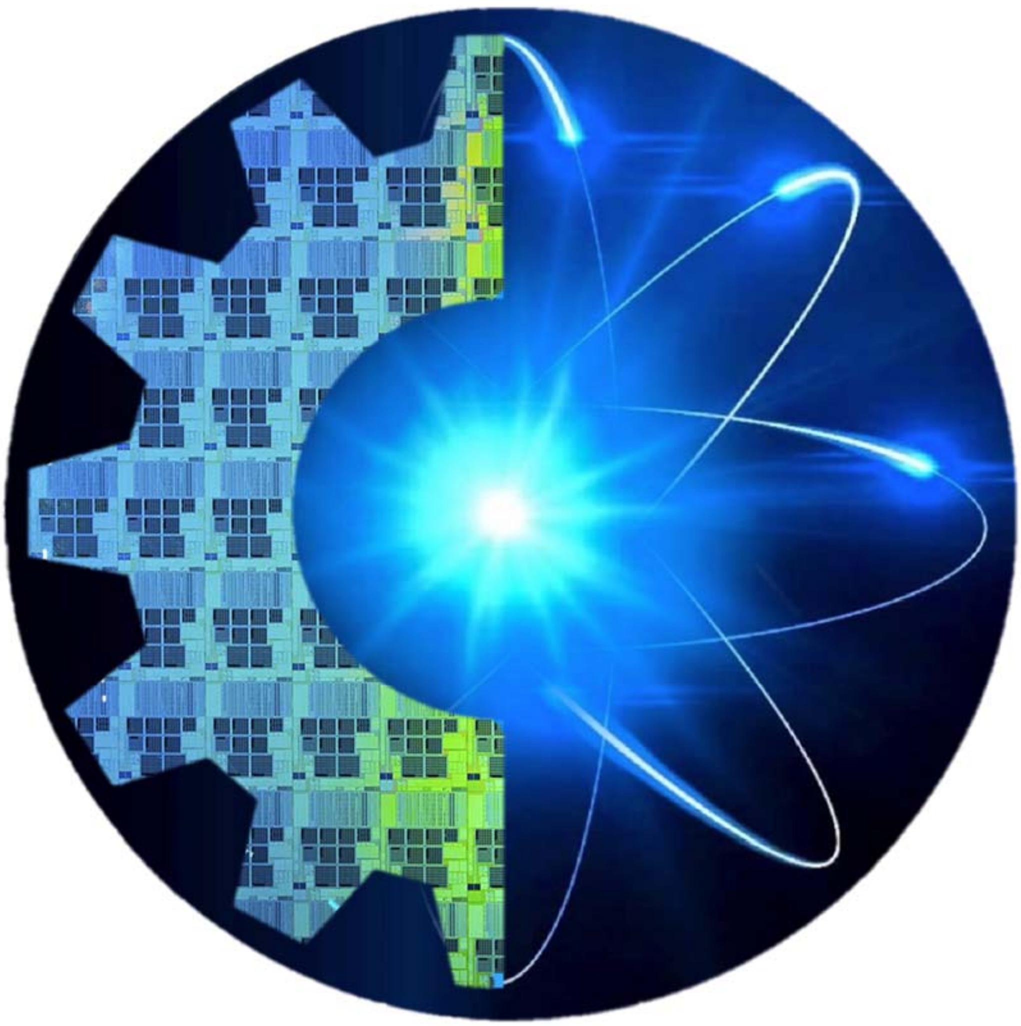
Department of Energy Office of Science
Fusion Energy Sciences Workshop

Plasma Science for Microelectronics Nanofabrication



Report on Science Challenges and Research Opportunities for Plasma Applications in Microelectronics

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Fusion Energy Sciences

Department of Energy Office of Science
Fusion Energy Sciences (FES) Workshop on
Plasma Science for Microelectronics Nanofabrication

Report on Science Challenges and Research Opportunities for Plasma Applications in Microelectronics

Based on a Workshop Sponsored by FES held, August 8-9, 2022, Gaithersburg, MD.

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Executive Summary

Low temperature plasmas are essential to the manufacture of devices in the semiconductor industry, from the creation of extreme ultraviolet photons used in the most advanced lithography to thin film etching, deposition, and surface modifications. It is estimated that 40-45% of all process steps needed to manufacture semiconductor devices use low temperature plasmas (LTPs) in one form or another. LTPs have been an enabling technology in the multi-decade progression of the shrinking of device dimensions, often referred to as *Moore's Law*. New challenges in circuit and device design, novel materials, and increasing demands to achieve environmentally benign processing technologies are pushing the boundaries of what is possible today in plasma technology.

The Department of Energy Office of Science Fusion Energy Sciences (FES) held a workshop titled *Plasma Science for Microelectronics Nanofabrication* in August 2022 to discuss the plasma science challenges and technical barriers needing to be overcome to continue to develop the innovative plasma technologies required to maintain and improve the internationally competitive US semiconductor industry. One of the key outcomes of the workshop was identifying a set of Priority Research Opportunities (PROs) to focus attention on the most strategic plasma science challenges to address to benefit the US semiconductor industry. For each PRO, scientific challenges and recommended strategies to address those challenges were identified. The PROs are listed below, each with a representative key question.

Priority Research Opportunities for Low Temperature Plasmas Used for Microelectronics Nanofabrication

PRO 1: Develop sustainable device manufacturing at extreme scales with integrated efforts in plasma science, reactor technology, process engineering, and plasma chemistry

Key question: *How can plasma-based manufacturing processes support the fabrication of cutting-edge devices while consuming less power and resources, and while eliminating the use and generation of global warming species?*

PRO 2: Advance understanding, characterization, and control of plasma-surface interactions down to the atomic scale to enable materials and device structures required for future microelectronics and semiconductor fabrication

Key question: *How do we independently optimize plasma-generated species fluxes and energies at wafer surfaces to control plasma-surface interactions at the atomic scale?*

PRO 3: Develop fundamental data and centralized databases to enable comprehensive low temperature plasma diagnostics and modeling

Key question: *How can the appropriate fundamental data for plasma modeling and diagnostics be rapidly produced to reduce plasma process development time?*

PRO 4: Enable experimentally validated, predictive, and integrated modeling of fundamental low temperature plasma physics, chemistry, and surface interactions to enable next generation semiconductor plasma processing

Key question*: What fundamental modeling and experimental validation capabilities, including new plasma diagnostics, are needed to enable predictive modeling of complex transient and multi-step plasma processing to reduce plasma process development time and complexity?*

PRO 5: Understand and control low temperature plasma generation of radiation, radiation transport and materials interactions in semiconductor processing systems

Key question: *How can plasma generated photons be used with minimal damage to advance* *nanofabrication objectives in both advanced lithography and processing?*

PRO 6: Develop novel institutional structures to meet emerging challenges of the field

Key question: *How can we develop new plasma technologies with both fundamental scientific and commercialization challenges while producing a workforce for U.S. industry that is knowledgeable about plasmas and their applications?*

1. Introduction

Since the 1960s, the model for innovation in the manufacture of semiconductor devices (e.g., microprocessors, memory chips) has been conceptually simple: double the number of transistors on a chip every 1.5-2 years with an ever-increasing performance to cost ratio. This industry guiding principle, known as *Moore's Law*, was inspired by an observation by Intel co-founder Gordon Moore. Low temperature plasmas (LTPs) have played an enabling and essential role in the progression of *Moore's Law* by enabling thin film deposition, etching and surface modification across entire wafer diameters with the precision, uniformity, and reproducibility required to advance device capabilities and sustain an internationally critical industry. LTPs also play essential roles in generating photons for the lithography that defines the patterns that are etched into wafers.

The importance of LTPs to the semiconductor fabrication industry, and thereby to the US economy, national defense, and energy infrastructure cannot be overstated. In the absence of LTP-enabled manufacture of microelectronics devices, we would have no computers, no cell phones, no "big data", no detection of black holes, no remote sensing, no world-wide-web, no modern medicine, no gene sequencing, no Webb telescope, no electronic publishing, and no autonomous vehicles. With LTP-enabled microelectronics, we have all of these things and more. The energy, defense, and economy strategies being pursued by the US are predicated on continuing advancements in LTP-enabled manufacture of semiconductor devices. To fulfill those plans, investments in plasma science, and LTP science in particular, are required.

Due to physical limits, the process of shrinking the dimensions of semiconductor devices is becoming increasingly more challenging and expensive, prompting the development of new device designs and architectures. These new devices and architectures will require new materials and new methods of fabrication, 3-dimensional (3D) heterogeneous integration, and fabrication at the atomic scale. The industry goal is to continue to achieve steady improvements in device performance while reducing costs, to reduce energy consumption in both manufacture and operation, and to minimize the industry's environmental impact, such as reducing greenhouse gas emissions.

Maintaining a robust and expanding an internationally competitive domestic microelectronics supply chain will require major new investments in semiconductor chip manufacturing capacity, enabled by advances in the supporting science and technology. One of the most important enabling technologies in microelectronics manufacturing is rooted in low temperature plasma science and the associated materials science and surface science that plasma activated processes enable.

The DOE Office of Science 2018 Basic Research Needs (BRN) study on Microelectronics [1] cited the challenges associated with continuing to improve computing power in the manner driven by *Moore's Law*. As the report cites, achieving this goal will require new materials, new synthesis technologies, and new circuit architectures and algorithms, all developed using co-design principles. To address the challenges and key questions discussed in the BRN, the plasma-based fabrication techniques that underpin the industry and the majority of materials synthesis processes must be integrated into the co-design process. The *Plasma Science for Microelectronics Nanofabrication* workshop prioritized the science challenges that must be addressed to enable that integration.

It is in this context that this report on plasma science for microelectronics fabrication was written. Low temperature plasma has proven itself over the decades to be an essential tool for scalable, economical, and ultra-precise microelectronics fabrication. This report outlines the nature of the emerging LTP science challenges and defines a set of priorities in plasma science research to meet the industry's challenges with new generations of plasma-based technologies. A workforce trained in these intrinsically multidisciplinary, plasma focused fields will be essential in maintaining US leadership in this indispensable technology, and the report addresses strategies to address workforce challenges.

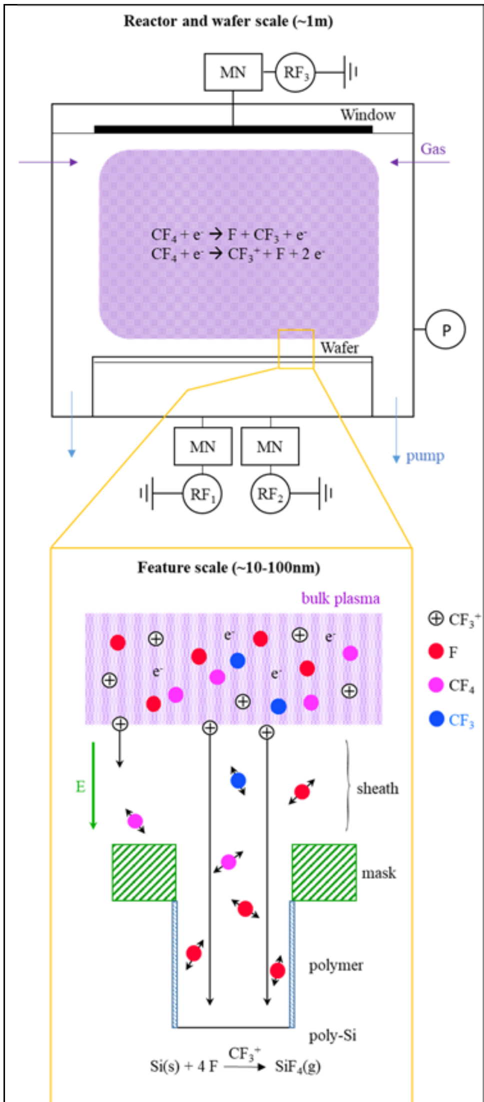


Figure 1: Si etching using a CF_4 plasma.

Figure 2: High aspect ratio structures fabricated using plasma etching. [173]

Low Temperature Plasma Etching of Semiconductors: Plasma etching is a critical technology that enables semiconductor device fabrication. In plasma etching a semiconductor wafer is placed in contact with a low temperature plasma with the goal of removing one or more materials from surfaces selective to other materials, and do so with nanometer resolution. During the fabrication of a typical integrated circuit, plasma etching is used dozens of times to make the intricate patterned structures in various dielectric, semiconductive, and conductive thin films that constitute microelectronics devices. Materials are etched by the plasma generating neutral radicals, energetic ions, and a combination of the two, which is known as reactive ion etching (RIE). These radicals and ions diffuse or drift to the wafer surface, reacting with surface species to remove material. As demonstrated in the classical experiment by Coburn and Winters [8], etching occurs more effectively when both ions and radicals contribute synergistically to material removal.

Etching is performed in low pressure plasmas (tens of mTorr to a few Torr) sustained in reactive gases such as Cl_2, O_2, or CF_4. (See Figure 1.) These plasmas are generated using techniques such as inductive coupling, capacitive coupling, or microwaves. These techniques control the variety and fluxes of ions and reactive radicals that strike the wafer. Photolithography is used to produce masks on the wafer having openings that define where the etching occurs. Methods have been devised to control the energy of ions striking the wafer. Most industrial plasma etching systems have provision for pulsing of radio-frequency power, which enables control of plasma properties on millisecond timescales. For some etching applications, the ions are filtered from the plasma and etching is only done using reactive radicals.

Low temperature plasmas offer many advantages that make their use essential for etching. Foremost amongst these are the unique capabilities to control both anisotropy and selectivity. It is these plasma-enabled capabilities that have allowed microelectronics devices to realize *Moore's Law* and continuously drive power, performance, and area improvements over the last 4 decades. Plasmas produce ions, whose energy onto the wafer can be readily controlled using electrical means. Sheaths at the plasma-material interface are used to direct ions vertically towards the surfaces, enabling anisotropic etching and the fabrication of small tightly-spaced structures (Figure 1). Reactive species can be produced in plasmas through electron-impact dissociation at low gas temperatures. This enables control of selectivity through careful selection of processing conditions, as well as etching materials without damaging the devices and structures that have already been fabricated on the wafer. In addition to chemically reactive species that contribute to etching, the plasma can also deposit films that shield surfaces from reactive species, thereby improving selectivity and anisotropy.

Two applications are pushing plasma etching to its physical limits. Etching with energetic ions can damage the near-surface region, necessitating the use of softer techniques such as atomic layer etching that offer atomic-scale precision. At the other extreme, etching of high aspect ratio (AR) features (AR > 100) requires highly directional ions having energies of 10 keV or more (Figure 2).

Relation to the DOE Office of Science and Fusion Energy Sciences Mission

Fusion Energy Sciences (FES) within the DOE Office of Science (SC) has an extensive portfolio that encompasses the range of plasma science and application – from high energy density and fusion science, to low temperature plasmas and their many applications. FES has recently completed a strategic planning process culminating in a report authored by FESAC (Fusion Energy Sciences Advisory Committee) titled *Powering the Future: Fusion and Plasmas*. [2] The report addresses the challenges and opportunities for bringing fusion power onto the electrical grid, while also addressing non-fusion priorities of FES in translating advances in fundamental science in low temperature plasmas to technologies for benefiting society. Relevant passes from the report include:

> *The Plasma Science and Technology area should focus on new opportunities to advance fundamental understanding and, in turn, translate these advances into applications that benefit society...Create Transformative Technologies. Unlock the potential of plasmas to transform society.*
>
> *A plasma-based technology research program will provide the scientific basis to enable the next generation of technological inventions. Plasmas can enable transformative technologies in manufacturing, microelectronics, biotechnology, medicine, and aerospace. Fulfilling this potential will require a dedicated, nimble research program able to take advantage of the translational nature of this research by connecting the basic science with the breadth of applications.*
>
> *Recommendation: Provide steady support for fundamental plasma science to enable a stream of innovative ideas and talent development that will lay the scientific foundation upon which the next generation of plasma-based technologies can be built.*
>
> *Recommendation: Establish a plasma-based technology research program focused on translating fundamental scientific findings into societally beneficial applications.*
>
> *Recommendation: Support research that supplies the fundamental data required to advance fusion energy and plasma science and engineering.*
>
> *The need for PPPs [public private partnerships] in the semiconductor arena in particular was highlighted in the 2020 decadal study...focused on breakthroughs in the 5- to 10-year time frame to strengthen US leadership in this trillion-dollar market. This incubator would involve collaborative activity between academia, startups, and established companies, with the end goal of advancing research and disruptive breakthroughs for the purpose of commercialization.*

Goals of the Workshop

The FES Strategic Plan makes clear the high priority of translating advances in fundamental low temperature plasma science to technology breakthroughs that benefit society. Low temperature plasma processing of microelectronics devices, an underpinning technology supporting the US semiconductor industry, aligns with those priorities. Participants in the workshop aimed to articulate the role of the DOE Office of Science, and Fusion Energy Sciences in particular, in advancing the plasma science required for new plasma-based semiconductor nanofabrication technologies. The major outcome of the workshop is a set of prioritized research opportunities (PROs) that can inform future research efforts in plasma-associated semiconductor nanofabrication science and build a community of next-generation researchers in this multidisciplinary area. Among the additional objectives of the meeting were:

- Identify the fundamental plasma science areas (and their challenges) that are now supported or that could be supported by FES that will advance semiconductor nanofabrication capabilities in this strategic industry.
- Correlate the current research strengths supported by FES with semiconductor nanofabrication applications with the goal of prioritizing research activities in FES mission areas, including discovery plasma science, identifying where new capabilities are needed and where partnerships could be beneficial.

- Identify related areas of plasma science and plasma materials interactions that would benefit from a research program focused on the plasma science for semiconductor fabrication.
- Define plasma science's role in the co-design process required to vastly increase computing power.
- Propose a roadmap for supporting investigation of these science challenges and possible partnerships that will result in their translation to practice.

2. Priority Research Opportunities (PROs)

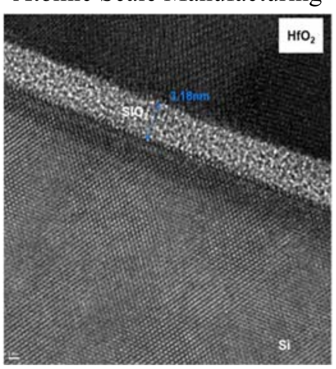
PRO 1: Enable sustainable device manufacturing at extreme scales with integrated efforts in plasma science, reactor technology, process engineering, and plasma chemistry

Sustainable fabrication of cutting edge nanoelectronics devices requires plasma assisted processes that can construct these devices with features manufactured at the atomic level alongside features that are 100s of atoms wide and 10s of thousands of atoms deep (see Figure 1-1). To manufacture devices at these extreme scales, basic plasma science, plasma chemistry, reactor technology, and process engineering must converge to formulate new plasma source concepts and accelerate their deployment to volume manufacturing for cutting edge devices. Exploration of new methods of plasma generation, new chamber components, and new process gases is essential for the fabrication of advanced devices with reduced energy consumption and minimal environmental impact. Toward these goals, an integrated research effort that extends from basic plasma science to advanced manufacturing technologies that enables co-design of hardware with manufacturing processes and lowers the barrier for industry collaboration with research institutions is needed to rapidly advance basic plasma science concepts to plasma reactor systems and manufacturing lines.

1a. Summary

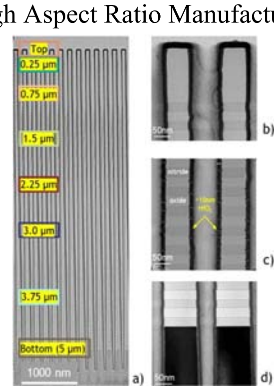
The equipment in which plasma assisted manufacturing is carried out for critical semiconductor processes is complex, expensive, energy intensive, and requires exotic feedstock gases that include greenhouse gases. In spite of these challenges, plasma processing is also the most easily scalable and economical technology for the fabrication of atomic scale and high aspect ratio features that define the devices that drive the semiconductor industry. Plasma etching and lithographic patterning are two of the most complex unit processes in the manufacturing flow for integrated circuits and are also the process technologies that

Atomic Scale Manufacturing



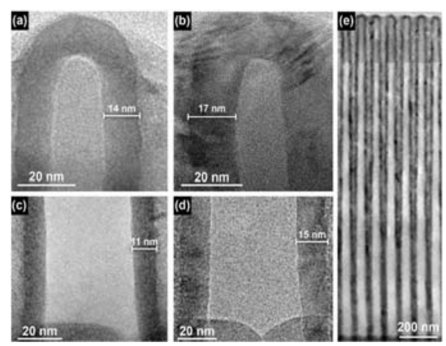
High-resolution transmission electron microscopy (HRTEM) image of the cross section of a HfO_2 thin film [168]

High Aspect Ratio Manufacturing



Cross section of a full 96 pair ONON stack with post-ALE measurement locations after HfO_2 deposition (a). Close-up of the same ONON structure at top of the stack (b), mid-section (c), and bottom (d) [167]

Challenging Geometry & Atomic Scale



TEM of high aspect ratio trenches (a) and (b) show top end of trenches coated with TiO_2 using thermal ALD and PEALD. (c) and (d) show bottom end of trenches coated with TiO_2 using ALD and PEALD. (e) TEM at lower magnification illustrates the high aspect ratio. [166]

Figure 1-1: What is "extreme scale" manufacturing and how does plasma processing contribute in this area? Cutting edge electronic devices are a combination of (left) atomic scale layers and (middle) challenging geometric features such as high aspect ratio structures, often combined together to form devices (right). The fabrication of these layers and these structures require very different plasma conditions that are increasingly having to work in synergy for advanced devices. This is the challenge for next generation plasma systems.

have defined the pace of *Moore's Law* more than any other process technology in high volume manufacturing (HVM). Plasma deposition and plasma surface modification also play key roles in semiconductor manufacturing.

Advancing plasma assisted process technology and the associated equipment used to fabricate nanoscale devices will be underpinned by advances in plasma science. These advances need to address the convergence of the continued scaling of *Moore's Law*, many novel materials, and the increasingly complex geometries of advanced devices and circuits. There is a need for plasma science to address the complexity and cost of these systems to make future manufacturing processes for microelectronic devices more efficient, environmentally friendly, and economical. Plasma assisted manufacturing of semiconductors has long benefited from the high dollar value of the finished product, enabling tolerating relatively high energy consumption, significant greenhouse gas (GHG) emissions, and relatively high operating costs. For semiconductor manufacturing in the US to regain a competitive advantage with manufacturing in other regions, science advances translated to technical solutions that address these issues are needed.

The supply chain and product life cycle of plasma manufacturing technology needs to be better positioned to provide solutions to these challenges. Infrastructure that supports co-design across the technology life cycle translating fundamental research to manufacturing as well as co-design across disparate plasma applications are needed to decrease the time from concept to deployment.

Advancing the plasma science upon which plasma reactor technology is based with the goal of speeding the pace of reactor technology deployment is critical for a competitive semiconductor manufacturing sector in the US. There are simply no competing technologies to displace plasma processing in the fabrication of microelectronics devices. Therefore, it is a manufacturing imperative that advances in integrated plasma science and engineering be translated to practice to improve process capability, sustainability, and time to market in order to maintain and solidify leadership in semiconductor manufacturing technology.

1b. Key Scientific Questions

The key scientific questions for this PRO span basic science, engineering challenges, and the deployment of technical and administrative infrastructure that will enable science discovery and accelerate translation of science advances to technology.

1. *What is the ideal combination of reactive species, charged particle, and photon fluxes for processing materials at extreme scales?*
2. *What techniques can be employed to generate, control, and monitor plasma generated fluxes (chemistry, charged particle, and photons) that advance science understanding while translating to the manufacturing environment?*
3. *How can plasma-based manufacturing processes support the fabrication of cutting-edge devices while generating minimal production of global warming byproducts?*
4. *How can plasma-based manufacturing processes support the fabrication of cutting-edge devices while consuming less power and less scarce resources then the current state of the art?*
5. *Can the semiconductor manufacturing technology development paradigm be reimagined to enable cooperative design from the basic science phase to the high volume manufacturing phase?*
6. *Can the supply chain for manufacturing systems be similarly reimagined to reduce or eliminate the decoupled science and technology advancement efforts between suppliers and equipment users?*
7. *Can these shifts be realized through the implementation of efforts similar to those currently in the DOE-FES portfolio such as the INFUSE program, LaserNET, and MagNET?*

1c. Scientific Challenges and Research Opportunities

1. Optimization of plasma generated fluxes for processing at extreme scales

At its core, the optimization of semiconductor manufacturing processes centers on the controlled delivery of chemically reactive species with optimized energy to the material surface, coupled with a high level of control over substrate temperatures. Low temperature plasma assisted manufacturing processes bring a singularly unique combination of these three elements. The reactive species are formed primarily through dissociation of gas phase molecules through electron collisions. These electron impact collisions enable reactive species production at low temperatures compared to traditional means. Energy delivery takes the form of electrons, energetic ions, excited atomic and molecular species, and photons that are formed in the non-equilibrium plasma. The ions also undergo anisotropic acceleration in the sheath that borders the plasma, and adjacent to the wafer in particular, providing the highly directional energy deposition that enables the fabrication of nanometer-sized features. The first step in designing an optimized plasma reactor for critical fabrication processes is to understand the LTP provided combination of chemistry and energy that will enable these manufacturing processes at extreme scales.

There are basic low temperature plasma science challenges that can contribute to the advancement of semiconductor manufacturing processes. Our understanding of the interaction between plasma generated species must couple the “plasma scale” (up to a meter) and to the “feature scale" (now, a few nanometers (nm) and shrinking). Currently these scales are treated relatively independently of each other and their coupling needs to be better understood. For example, surface reaction kinetics involve novel plasma generated species, which change the boundary conditions for the plasma. The synergy of plasma species in surface reaction kinetics needs to be more completely understood. The synergy of photon, electron, and metastable species interactions with surfaces should be understood at the same level as ion interaction with materials. As device dimensions shrink to atomic scale manufacturing, damage becomes more sensitive to the energy ions accelerated in the sheath. Future generations of devices may be able to leverage these other plasma species to contribute or replace the benefits now received from energetic ion fluxes. These synergistic processes need to be better understood.

The ability to form high aspect ratio (HAR) features is a unique strength of low temperature, non-equilibrium plasma processing. As the aspect ratio (height over width) increases, the usual response is to increase the energy of ions incident into the feature to reach the bottom of the feature, which translates to higher voltage applied to the substrate. These process trends have strained hardware capabilities, with current voltages already well over 10kV. With these processes being ion-flux dominant, addressing these challenges encourages tailored ion energy distributions, pulsed plasma source, and remote plasma source generation of reactive species. The goals include extending HAR processes to greater depths as well as minimizing feature shape distortions such as tilting, twisting, and sidewall distortion.

To achieve higher aspect ratio features for next generation devices, more efficient delivery of plasma energy to the bottoms of these remarkably deep and narrow features will be required. This challenge requires understanding how energetic species (ion, photon, or otherwise) interact with the new materials of interest. This includes controlling complex plasma transport to the feature, in the feature, and surface chemical reactions within the feature.

In contrast with etching HAR features, controlling surface processes at the atomic scale generally requires much lower energies at surfaces. For example, ions impacting surfaces at even a few eV can produce atomic scale point defects. This trend works against the desire to have large fluxes of ions to speed processing – more power typically means more energetic ions. Atomic layer deposition (ALD) and atomic layer etch (ALE) processes generally operate in a cyclic fashion which is generally slow. Developing plasma processes that are compatible with this cyclic operation delivering soft energy to surfaces yet are rapid are needed. Understanding plasma transport that addresses both high aspect ratio and atomic scale processing is needed to enable high process rates, across-wafer uniformity, and minimal edge exclusion (area at edge of the wafer that does not produce useful devices).

2. Optimizing plasma generation for cutting edge sustainable processes at extreme scales

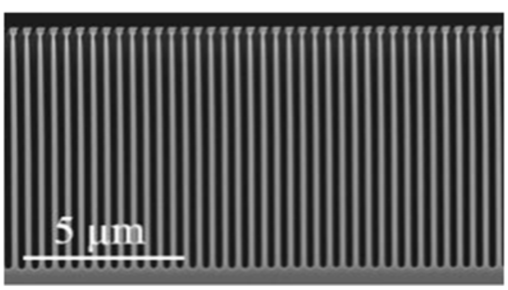
The needs for low temperature plasma assisted manufacturing of next generation microelectronics devices are novel plasma generated chemistries and energetic species control that do not reduce manufacturing productivity and are scalable to manufacturing levels. Meeting these needs will require advances in basic plasma science translated to scale up and deployment.

Novel plasma chemistries are produced by a combination of choice of the working gas and controlling the energy distribution of electrons that collisionally dissociate these molecules (and their dissociation products). At the reactor level, finding new pathways to manipulate the electron energy distribution can present novel dissociation pathways for new chemistries. This control becomes increasingly more important as now commonly used processes gases that have significant global warming potential are phased out. This transition in feedstock gases will require novel methods of replicating plasma chemistry compositions that match current conditions with different feed gasses.

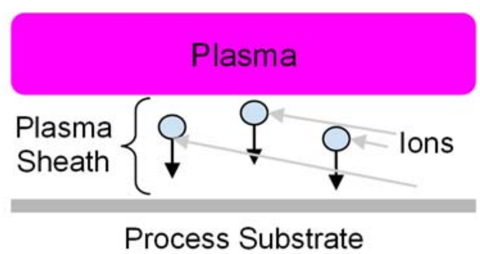
Energetic species control centers on manipulating the electric potentials and fields that naturally form in bounded low temperature plasmas. Time modulation of power and processes present new scaling relationships between species energy and processing metrics, where short periods of high energy fluxes are combined with periods of low energy fluxes. The emergence of pulsed plasma processing suggests that some overlap may exist between the traditionally decoupled "high energy" and "low energy" process modalities. [3]

The formation of features with challenging geometries such as HAR features can be realized only through anisotropic (vertically directed) ion bombardment of the substrate. Both average ion energy and ion energy distribution functions are largely controlled by the application of time varying potentials to chamber surfaces. As etch features grow in aspect ratio, a general trend has been to increase the average ion energy proportionally so that the ions can reach the bottom of the feature (see Figure 1-2).

By contrast, in atomic scale manufacturing, the processes of film deposition and etching tend to be driven more by neutral species chemistry. Energetic species such as ions, electrons, and photons must be managed to provide a relatively 'gentle' surface reaction enhancement. Reduction of the sheath potential above the wafer as well as the positive plasma potential that naturally forms between surfaces and the bulk plasma are needed to ensure charged species energies incident onto the wafer are below the displacement energy for surface atoms. This tends to require lower electron temperature to keep these bulk and periphery



HAR profiles in Si [161]



Conceptual diagram of plasma sheath

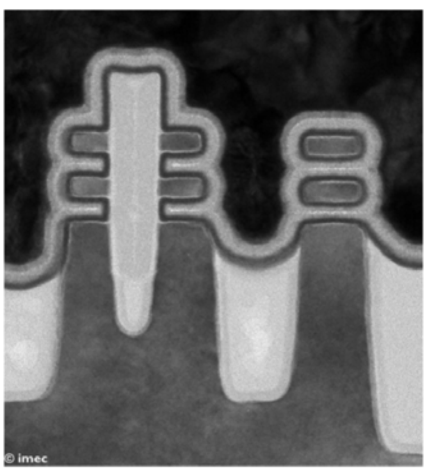
Figure 1-2: Ion delivery for high aspect ratio features: manufacturing trends and science challenges. (left) The fabrication of extreme high aspect ratio features (HAR) requires directional fluxes of energetic ions into these features to provide energy for plasma activated removal of material at the bottom of the structure. Typically, to form deeper features higher ion energies are required. This has long been a trend in semiconductor manufacturing. (right) These high energy ions are formed in the plasma and accelerated through the sheath at the surface of the wafer. The ion path remains largely perpendicular to the substrate surface as long as the ions do not collide with neutral gas atoms in the sheath region. The electric potential V that accelerates the ions is formed in the plasma sheath. The size of the sheath increases with $V^{3/4}$, therefore the probability of ion collision (and less anisotropy) also increases with increasing voltage. This further increases the challenge of providing sufficient ion flux to the bottom of these features. The plasma and feature scale lengths must be linked to optimize these processes.

potentials to a minimum. Although this strategy works well to minimize accelerating potentials, it presents manufacturing challenges such as increased process sensitivity to process setpoint variability. (See Figure 1-3.)

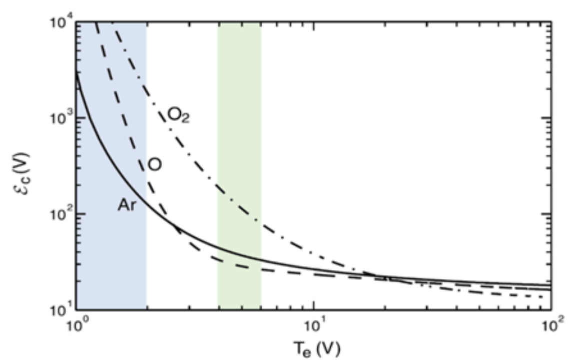
Along with controlling plasma properties to selectively generate chemically active species, exploration of plasma driven surface processes at extreme conditions such as cryogenic temperatures have also shown promise. A better understanding of surface interactions with plasma species at these low temperatures could open additional opportunities for advanced plasma assisted manufacturing. [4]

Developing new plasma sources will require improved ability to control fundamental plasma properties and will also require improved sensor and control algorithms. The plasma conditions that produce optimum reactive fluxes are also the conditions that have the most variability and instabilities. Sensors and control algorithms are required to maintain the desired plasma properties. Although plasma chambers can be designed around sensors for scientific studies, any plasma control method for manufacturing requires integration into manufacturing platforms without increased cost or impact on process performance. Information must be processed sufficiently rapidly that real-time or near real-time control is achievable. Despite the increased complexity of process recipes, computational speed is approaching a level where simulated results and sensor inputs could provide a path for process emulation on the millisecond timescale. This might enable process re-optimization and "emulation on the fly."

In addition to direct contributions of LTPs to materials processing, LTPs have long served a fundamental role as a photon source in lithography, beginning with Hg-arc lamps through excimer laser, and now as extreme-ultra-violet (EUV) lighting sources. Low temperature plasmas have also moved into new applications such as medicine and agriculture due to the development of more stable sources that can run



TEM image of IMEC 17 nm forksheet FETs, featuring atomic scale processes alongside both vertical and horizontal anisotropic etch processes. [169]



Collisional energy loss per electron-ion pair created as a function of electron temperature [164]

Figure 1-3: Atomic scale processes need a "gentle" plasma. What manufacturing challenges does this present? Fabrication of atomic scale features (left) requires plasma components that are energetic enough to initiate reactions, but gentle enough not to generate undesirable defects and damage. Specifically, the energies of incident ions need to be well controlled, and electrical potentials in the plasma need to be low to enable this. These ideal conditions tend to occur at lower electron temperatures (nominally 1eV-2eV) compared to traditional plasma processes (nominally 4 eV-6 eV). Achieving such fluxes typically makes a plasma reactor more sensitive to variability in process conditions. An example (right) is the change in required energy for electron-ion pair formation in the gas phase for low electron temperature (blue) and currently employed temperatures (green). This parameter establishes plasma density, rate of reactive specie production, and other critical process conditions. As electron temperature drops, this parameter becomes much more sensitive to comparable variation in temperature, increasing the demands on process control, monitoring, and reproducibility. Discovering pathways to better manage and control this increase in variability will be critical for next generation manufacturing.

at atmosphere pressure. Under atmospheric conditions, plasmas in semiconductor processing could play a role in liquid processing and multiple steps in surface preparation/cleaning.

3. Elimination of global warming byproducts in plasma processes

Plasma processing of semiconductors has historically relied on gas feedstocks that are not necessarily environmentally friendly. These may not be available in the future. Perfluorocarbons, hydrofluorocarbons, and other gases with greenhouse potentials many orders of magnitude greater than carbon dioxide are common feedstock gases for plasma etching. Helium is commonly used as a process gas and for wafer backside substrate cooling but is becoming increasingly expensive due to scarcity. Scarce resources such as helium will need to be replaced with alternatives, or methods for resource recovery and reuse will be needed.

It is expected that currently used plasma process gases with high greenhouse potentials will be phased out of manufacturing. [5] Fluoroether compounds have shown promising process enhancements with lower greenhouse potentials. [6] Developing new plasma sources, plasma chemistry and understanding plasma transport with these new families of gases that are more environmentally benign is a high priority for the industry. Plasma based reactor exhaust abatement is a well-established technology that is currently built into newer manufacturing facilities; however the current plasma-based technologies have several limitations. Development of high efficiency environmentally benign plasma abatement solutions would reduce GHG emissions from manufacturing facilities.

4. Improved sustainability for plasma processes

Plasma processing of semiconductors often requires high levels of energy consumption. The electrical power per unit area of wafer has increased over threefold in the last two decades. As power requirements continue to increase, alternative technologies that were previously too energy intensive for high volume manufacturing will likely become viable. For example, plasma processing with the wafer at cryogenic temperatures has historically been energy intensive compared to standard plasma processing technologies. However, cryogenic process energy costs may soon be lower than traditional process technologies when applied to emerging etching challenges.

Plasmas for semiconductor processing are generated and sustained by plasma power supplies. Individual plasma etching reactors may have 2 or 3 separate power supplies delivering a total of 10 -30 kW, and there might be several hundred of such reactors in a single fabrication facility. Efficiencies of these power supplies have improved over the last decade, but additional efficiencies could be realized to make the overall process more sustainable. An important aspect of developing more efficient power supplies is to understand the manner in which power is transferred into the plasma and creates an impedance to which the power is delivered – ultimately matching power deliver to consumption. Improving our ability to craft plasmas that both produce the needed radicals and ions, while also being capable of efficiently receiving power would greatly improve the sustainability of plasma processing.

5. Leveraging co-design to advance plasma reactor development for manufacturing, reliability, and technology capability

The development of semiconductor manufacturing technologies, including plasma assisted manufacturing, is to a large extent isolated in their individual disciplines. Advances in manufacturing technologies suffer from barriers to co-design, from concept to high volume manufacturing products. Concepts for new plasma sources typically begin at the tabletop scale, often in universities and national laboratories. However, scale-up of plasma source technologies for manufacturing is usually best done by equipment suppliers. Co-design of plasma reactors between university research centers and the semiconductor equipment manufacturers would accelerate the transfer of new plasma source technologies to the manufacturing floor. Similarly, plasma and surface diagnostics development at the research level tends not to consider the challenges of integrating new technology into the manufacturing environment. Industry engagement at the research phase of these diagnostics would accelerate the practical introduction of new process monitoring technologies in manufacturing.

Due to practical matters of cost and facility, plasma research teams in universities and national laboratories generally investigate LTPs and develop new plasma reactors on platforms that do not have the full suite of processing subsystems that are needed to demonstrate advances in plasma processing at state-of-the-art scales. For example, gas handling, substrate temperature control, cleanliness, and advanced metrology are not typically available on the research reactors used to investigate fundamental processes. As a result, advances in plasma science developed on those systems do not necessarily directly translate to practice. Closer collaboration between university and national laboratory research teams and industry will speed the translation of advances in fundamental plasma science to new reactor concepts in manufacturing. Co-design between plasma applications (PECVD, PVD, etch) also presents significant opportunities for accelerated technology deployment.

Existing DOE programs that promote synergy between universities, national labs and industry can serve as a model for promoting co-design in transitioning LTP science to applications. Within DOE-OFES, the INFUSE program is designed to accelerate new fusion technology by encouraging collaboration between companies, the DOE laboratory network, and universities. In 2022, INFUSE supported 18 projects that connected 10 companies, 8 universities, and 3 DOE laboratories in collaborative research projects. [7] Programs such as the NSF GOALI and I/UCRC programs promote academic/industry research collaborations. These programs are models for increasing collaborative research in plasma assisted manufacturing. The DOE supported network LaserNET-US and the emerging MagNET-US network have reduced barriers to research facilities and opportunities for critical workforce development. The LTP cooperative research facilities at Princeton Plasma Physics Laboratory and Sandia National Laboratory have similarly provided access to world class diagnostics and simulation resources to the broader LTP community. These three research networks are potentially well aligned with the research needs of the plasma nanomanufacturing community. Further discussions of needed changes to institutional structures are provided in PRO 6.

1d. Potential Impacts

Advances in science of LTPs and plasma surface interactions are critical to the development of high volume manufacturing of semiconductor devices that are less energy intensive, more sustainable, and more friendly to the environment. The potential impacts of the efforts described here includes more rapid deployment of manufacturing reactor technology that provides efficient volume manufacturing solutions for devices at extreme scales while reducing the environmental impact of plasma processes. There will be concomitant savings in materials, energy, and overall cost. Increased collaboration between universities, national labs, and industry will accelerate scale up of laboratory scale plasma science investigations to advanced manufacturing. Increased synergy across the supply chain, from power supplies to reactor diagnostics, will increase co-design and co-development efforts from the component level to the optimization of the final manufacturing process. Speeding the translation of advances in LTP science requires mechanisms for co-design of new reactor concepts, technology, processes, and diagnostics from the fundamental research phase through industrial implementation.

PRO 2: Advance understanding, characterization, and control of plasma-surface interactions down to the atomic scale to enable materials and device structures required for future microelectronics and semiconductor fabrication

2a. Summary

Low-temperature chemically reactive plasmas are used for depositing and etching semiconductor, dielectric, or metal layers and creating circuit features that are as small as a few nanometers. Plasmas also emit light from the vacuum ultraviolet (VUV) to the infrared (IR), and these photons impinge on all plasma facing surfaces. Consequently, a deep and fundamental understanding of how plasma-generated energetic and reactive species interact with material surfaces, both the wafer and the walls of the plasma chamber, is necessary to better control existing plasma deposition and etching processes and develop new ones.

This need to understand plasma-surface interactions is not limited to surfaces on the wafer and the materials in the integrated circuits. For example, plasmas used in microelectronics and semiconductor device manufacturing are confined within chambers. Inevitably, plasma interacts with the chamber walls and all other bounding surfaces. These interactions of the plasma with chamber walls change the character of the plasma, thereby presenting challenges to reproducibility of the plasma process, and practical matters such as producing particles that may contaminate wafers.

Plasma-surface interactions refer collectively to interactions at the plasma-material interface (i.e., the topmost surface of the material in contact with the plasma) and the subsurface regions of these materials. The subsurface region may extend to several or even hundreds of nanometers below the surface. The depth of the interaction depends on the surface composition and structure of the material, as well as the composition and energies of all species impinging on the surface. For instance, ultraviolet photons (UV) produced by the plasma are absorbed approximately in the top hundred nanometers of a plasma facing material, and have energies large enough to break bonds, create defects, or initiate chemical reactions. Similarly, plasma produced ions impinging on the surface with energies of 10-1000 eV can induce bond breaking and promote other processes at least several nanometers below the surface. Damaged, porous, and roughened surface layers may allow radicals to diffuse and penetrate similar or greater distances into the materials exposed to a plasma. Thus, the surface should not be taken to mean a two-dimensional surface but a sometimes difficult-to-define region at the top of the material exposed to a plasma. Given that semiconductor devices now have features with dimensions as small as a few nm, it is critical to understand, and control, the fundamental processes occurring during plasma induced modification of those surfaces.

The atomic scale processes that occur in this near-surface region are diverse and complex. This diversity and complexity are brought about by the diversity of the plasma produced species impinging on the surface and their cooperative synergies that may be either beneficial for semiconductor processing or damaging. The research opportunities generally arise from the need to understand and control these plasma-surface interactions while leveraging the synergies between different species impinging on the surface to

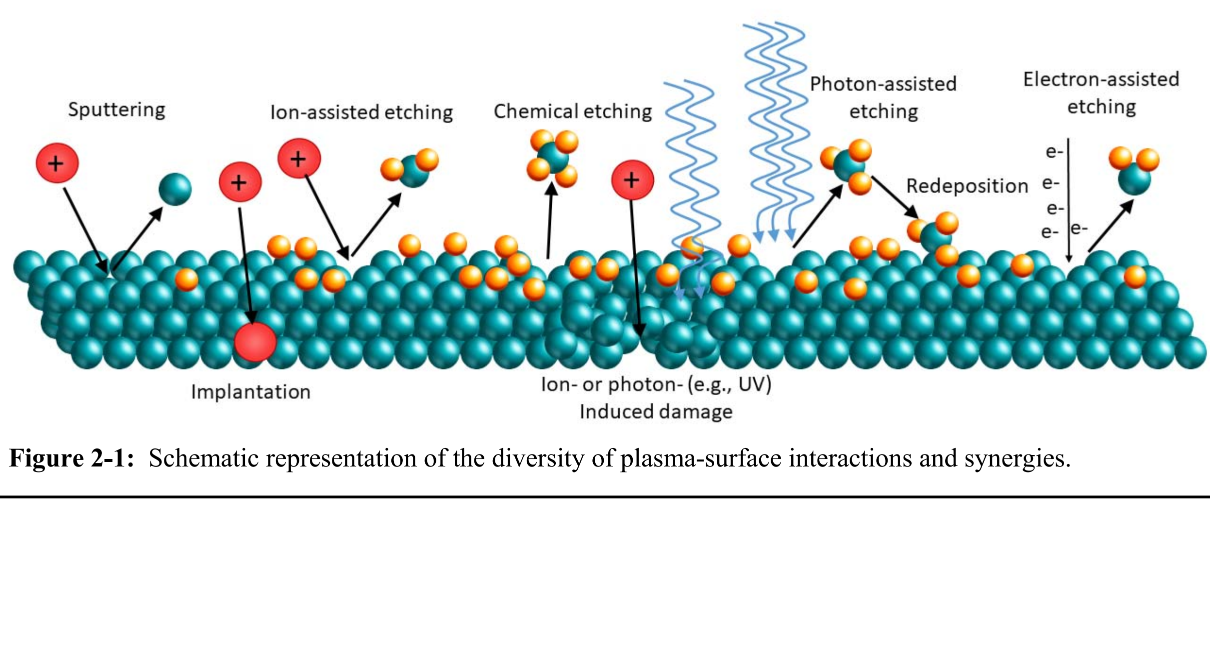


Figure 2-1: Schematic representation of the diversity of plasma-surface interactions and synergies.

create the device structures that are desired.

A schematic of different species produced in the plasma, impinging on the surface, and representative processes occurring on the surface of a material exposed to a plasma is in Figure 2-1. This material can be semiconductor, dielectric, metal, organic or inorganic, crystalline, or amorphous in microelectronics manufacturing. The diversity of materials used in microelectronics manufacturing, combined with the diversity of species that can be created in the plasma and impinge on the surface, results in an enormous number of possible plasma-material combinations.

2b. Key Scientific Questions

1. *How do we independently optimize neutral and ion fluxes for desired plasma-surface interactions at the atomic scale?*
2. *Are machine learning and artificial intelligence approaches applicable and adaptable for controlling, understanding, and optimizing plasma processing at the atomic scale?*
3. *What are the atomic scale mechanisms in plasma-enhanced atomic layer etching (PEALE), plasma–enhanced atomic layer deposition (PEALD), and plasma-enhanced area selective deposition (PEASD)?*
4. *How do we tailor plasmas, wall materials, and wall coatings to achieve precision, repeatability, and manufacturability for future leading-edge semiconductor and chip manufacturing technologies?*
5. *What new plasma processes are needed for emerging materials (e.g., EUV resists, spintronics, ferroelectrics, memory devices, etc.)?*
6. *How do imperfections (defects, dopants, etc.) get produced in microelectronics-relevant materials when immersed in plasma? How long do these imperfections reside on a surface?*
7. *How can plasma-enhanced atomic layer etching (PEALE), plasma–enhanced atomic layer deposition (PEALD), and plasma-enhanced area selective deposition (PEASD) be modified or enhanced for higher throughput and lower cost?*
8. *How do we study and understand fundamental factors such as determining purging and stabilization times, cycle times and time to self-limiting behavior in PEALE, PEALD, and PEASD?*
9. *How do we achieve true plasma-enhanced atomic layer etching?*
10. *How do we control the evolution of complex shapes and surface/interface profiles during plasma etching and deposition of 3-D complex structures?*
11. *How do we replicate plasma-surface interactions in hydrofluorocarbon plasmas that have been exploited in tailoring feature profiles and controlling selectivity with gases (or combinations of gases) that have lower or no global warming potential?*

2c. Scientific Challenges and Research Opportunities

The following is a non-exhaustive list of important challenges and research opportunities in understanding and controlling low temperature plasmas-surface interactions. Many of these challenges are coupled and addressing one can impact others. For instance, understanding and controlling synergies among the plasma species that impinge on the surface (e.g., neutrals, ions, electrons, and photons) is a challenge. Advances in this research field could impact the challenges of etching and depositing materials over selected areas one layer at a time with atomic layer precision as well as challenges in controlling defects at the surface and subsurface. The development of diagnostics and metrologies to quantify surface species, defects, fluxes, and energies would accelerate advances in all research areas.

1. Understanding and controlling the synergy among species that impinge on the surface

One of the challenges of understanding and controlling low temperature plasma-surface interactions is the complexity and the variety of ways plasmas can interact with materials immersed in plasma (for example, Fig. 2-1). Plasmas are comprised of electrons, ions, and multicomponent mixtures of neutrals, radicals, and ions, and these all impinge on surfaces with energies varying from 0.026 eV (room temperature) to hundreds or even thousands of eV. Their fluxes are widely varied depending on how the plasma is generated. Consequently, ratios of the fluxes of these difference species can be such that their effects on the surface are coupled. For instance, the synergistic effect of ions with neutrals and radicals on surfaces in the plasma etching and deposition of thin films has been well known and exploited for ion-assisted etching or deposition. [8] Other synergistic effects include those between photons and neutrals and radicals [9] (photo-assisted etching or deposition) and electron beam-assisted etching [10]. In some cases, there could be a three-way coupling between the effects of various species impinging on the surfaces in low temperature plasmas. The effect could synergistically enhance the etching rate or could be anti-synergistic. For instance, recently, anti-synergism between photo-assisted and ion-assisted etching was demonstrated. [11]

Designing and conducting well-defined experiments to reveal and quantify the coupling and (anti)synergy among the different plasma produced species impinging on the surface of a given material remains an important scientific challenge. Investigating the fundamental LTP-surface interactions that are important to semiconductor device fabrication is best performed under conditions that are as close as possible to those used in manufacturing. Although pristine beam-surface experiments performed under UHV (ultra-high-vacuum) conditions provide keen insights to fundamental processes, several decades of experience have shown that these results are difficult to translate to fabrication environments that have a variety of species and energies striking a surface. Conducting such fundamental experiments in the realistic environment of plasma etching or deposition equipment that are used in manufacturing is an even bigger challenge because such equipment typically does not have the access needed for the sophisticated spectroscopic equipment used in fundamental investigations. There is a continued need for surface diagnostics to interrogate the surfaces exposed to plasmas and to collect quantitative data for revealing the surface species, processes, and their rates either under conditions that closely mimic the plasma processing environments in plasma etching and deposition equipment or in situ in the actual equipment used in the manufacturing of chips.

Research is needed on how to independently control, vary, and optimize neutral, ion, electron, and photon fluxes to the surface. This capability is ultimately rooted in being able to control the energy distributions of these species in LTPs, both in the gas phase and incident on surfaces, often in a tight range, and vary them independently. More generally, there is a need to understand energy flow in low temperature plasma from the electromagnetic and electric fields used to generate the plasma to electrons, neutral molecules, ions, and photons and eventually to surfaces in contact with the plasma. Moreover, research is needed to determine the etching rates of materials relevant to CMOS manufacturing (e.g., metal oxides, silicon oxides, nitrides, photoresists, carbon, and other mask materials) and emerging materials (e.g., 2-D materials) processing under various combination of fluxes and energies. (CMOS – complementary metal-oxide-semiconductor – is the device architecture that currently dominates the semiconductor industry.) There is a need to expand the palette of mask materials in lithography that define the features to be etched to those that offer higher selectivity (less erosion) at lower aspect ratios. Finally, it will be important to understand how these synergies emerge and change as variables such as the surface temperature and the relative fluxes of ions, electrons, radicals, and photons are changed.

2. Addition and subtraction of materials to and from the surface one layer at a time over large areas: plasma-enhanced atomic layer etching and deposition (PEALD and PEALD)

Atomic layer etching (ALE) and atomic layer deposition (ALD) emerged from the need to control thin film deposition and etching at dimensions equivalent to adding or removing one atomic layer at a time. [12] Plasma-enhanced versions of ALE and ALD (PEALE and PEALD) bring additional flexibility and advantages, expanding the range of process variables and the variety of materials that can be deposited or etched. The steps in typical thermal and plasma ALD processes using the deposition of Al_2O_3 as an example are shown in Figure 2-2. PEALE is schematically shown in Figure 2-3. In atomic layer deposition or etching, the addition or removal of a single atomic layer of a film is separated into two half cycles, both self-limited in the sense that the reaction stops after a single atomic layer has reacted. For instance, in depositing Al_2O_3 film, the first half cycle is the exposure of the surface to the neutral precursor trimethylaluminum ($Al(CH_3)_3$, TMA) to adsorb a monolayer. This adsorption step is self-limited and stops after saturation coverage is reached. Subsequently, the surface saturated with TMA is exposed to an oxidizing environment in the second half cycle. In the case of PEALD, this may be a plasma containing water vapor that forms Al-O-Al bonds and leaves the surface saturated with OH adsorbates via reactions with H and OH ready for the first cycle to be repeated. In the case of PEALE of silicon, the two cycles are exposure of the surface to plasma produced Cl radicals to form a chlorinated surface followed by Ar ion bombardment of this chlorinated surface to remove the chlorinated silicon atoms.

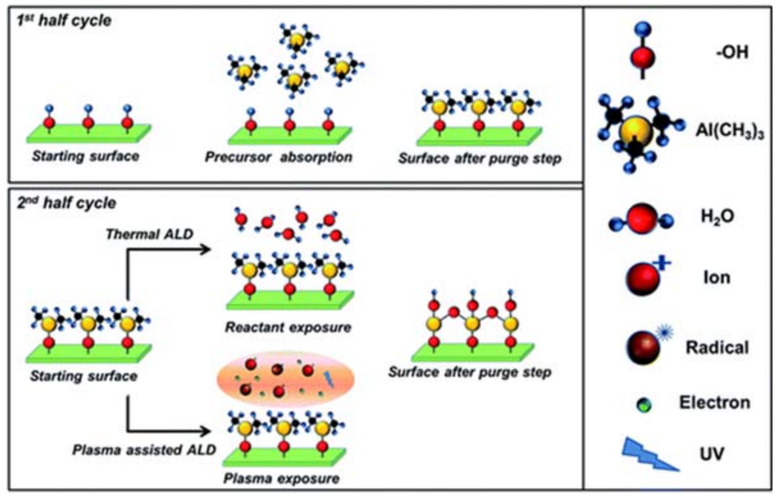


Figure 2-2: Illustration of the steps in the thermal and plasma assisted (enhanced) ALD for the deposition of Al_2O_3. [171]

Each cycle exposes the surface to the appropriate choice of neutrals, radicals, or ions to process the surface layer by layer. The synergies and reactions are separated into self-limiting steps to allow digital layer-by-layer etching or deposition of a material. One can add photons and electrons to the palette of species choices for deposition and etching in each cycle. This expands combinations of species that can be used to achieve the desired chemistry on the surface. It should be clear that understanding and controlling the synergies among the species created with plasma (ions, electrons, photons, radicals) can create tremendous opportunities in designing and developing PEALD and PEALE processes. To realize those opportunities, unprecedented control of LTP generated species onto the surface (fluxes and energies) is required. This control will in turn be realized by understanding and controlling the flow of power through the plasma and beneficially manipulating particle distribution functions.

Despite advances, the relatively slow throughput of PEALE and PEALD processes remains an enormous challenge. Each step typically entails pumping out the gases used in the prior step and refilling with the gases for the current step, and this purge-and-fill takes time. In addition to expanding the palette of PEALE and PEALD chemistries to etching and depositing emerging materials with new etchants and precursors, a better understanding of the fundamental surface reaction mechanisms is needed to increase throughput and efficiency. Important PEALE and PEALD process parameters such as purge and cycle times depend on the kinetics of plasma-surface interactions. There is a need for a better understanding of the interactions of plasmas with inhibitors and films for area-selective PEALD. (Area selective deposition is depositing on

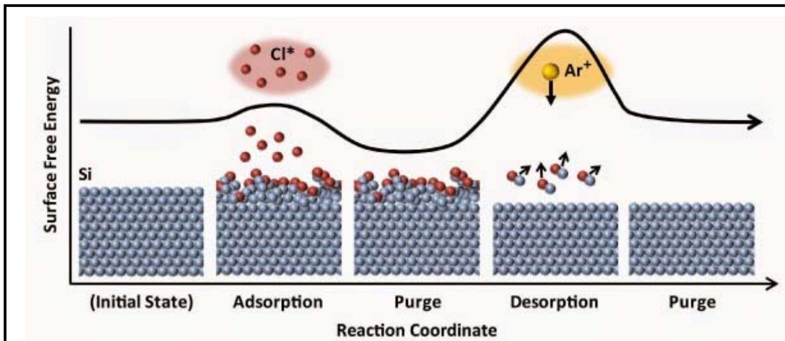


Figure 2-3: Illustration of typical steps in plasma enhanced atomic layer etching of Si (PEALE). [170]

one material but not an adjacent material only a few nm distant.) There is also a need for etchants and precursors with low global warming potential, as noted in PRO 1. New precursors are also needed for conformal gap filling using PEALD, where the film is deposited with a uniform thickness on a device having a complex shape. Research is needed to develop not only anisotropic but also isotropic PEALE processes. For instance, a new process is needed to replace the use of HF liquid etches with an alternative isotropic PEALE process to alleviate the safety concerns with HF.

3. Achieving true plasma-enhanced atomic layer etching (PEALE)

While plasma enhanced atomic layer etching is emerging in semiconductor manufacturing, removing the material one individual layer at a time while maintaining a smooth surface at the angstrom scale remains challenging. In true ALE, a self-limiting chemical modification step that affects only the topmost atomic layer is followed by an etching step that removes only these chemically-modified areas. In principle, repeating this cycle allows the removal of individual atomic layers one layer at a time. The classic example is the etching of silicon by alternating the adsorption of chlorine atoms to form a chlorinated surface and then removing this layer with energetic argon ion bombardment (Figure 2-3). The ion energies and the duration of the argon-ion exposure must be just right to remove only the chlorinated silicon atoms without roughening the surface or causing damage to the subsurface. Removal of only one monolayer per cycle of chlorine and ion argon exposure to achieve saturated and self-limited etching is difficult not only for the etching of silicon but also for other materials. In most cases, something that resembles this idealized situation is achieved by pulsing the plasma power and/or gases and is referred to as quasi-PEALE. The research challenge in achieving true PEALE is controlling the LTP produced fluxes and energies of reactive species incident onto the wafer surface with the reproducibility and precision that preserves the integrity of single atomic bonds. There is a need to develop PEALE processes that come as close to the self-limiting one atomic layer at a time etching as possible while still maintaining high throughputs. While this may not be absolutely necessary for etching relatively thick films (e.g., >10 nm), it will become necessary when monolayers or layered 2D materials must be etched with increasing atomic precision.

4. Plasma-surface interactions in plasma etching and deposition for 3-D integrated circuits

Increasing the area density (devices/cm^2) of transistor and memory cells has traditionally and still relies on shrinking the size of the devices. This has usually been done with a single plane of devices – 2D architectures. To achieve higher device densities, microprocessors and memory chips now stack devices in the third dimension. Vertically integrated 3D circuits increase device density, enable faster signal transmission, and provide flexibility for novel architectures and integration of logic and memory. As noted in PRO 1, 3D circuits require plasma etching of extremely high aspect ratio (HAR) features, a challenging task since ion and radical fluxes to the bottom of the feature change with depth and etching time. In addition, sidewall and bottom electrical charging inside the features by the electron and ion fluxes into the feature produce in-feature electric fields. These electric fields affect the fluxes and trajectories of ions and, therefore, how the etching profile evolves. The situation is also complicated because the fluxes and etch rates can depend on the adjacency of neighboring devices, the mask and material being etched, and the plasma chemistry. Therefore, there is a need to understand the coupling of LTP produced reactive species incident onto the side and bottom walls of the HAR features for plasma etching and deposition, and how to manipulate those fluxes to control in-feature processes.

Controlling the interaction of LTP produced reactive fluxes with the increasingly complex shapes of on-wafer features is essential. The control of manufacturing 3-D complex structures is a major challenge for the manufacture of devices, and fundamental plasma-surface interactions relevant to surfaces and materials structured from a few nm to microns should receive more attention. For instance, understanding ion deflection due to surface charging and redeposition of mask or etched material on sidewalls of features have always been important factors in determining the feature profile evolution. This importance will increase for 3D circuits and ever-increasing complexity of integrated circuits.

5. Interactions between plasma species and surfaces of emerging materials

While some plasma-material combinations such as halogen plasma etching of silicon or fluorocarbon plasma etching of silicon nitrides and oxides have been extensively investigated because of their technological importance, new plasma-material combinations are encountered in emerging fields where virtually no information exists regarding their plasma-surface interactions. In addition to the need for a more detailed understanding of plasma-surface interactions for CMOS materials, there will be a need for a deeper understanding of plasma-surface interactions for all plasma-material combinations that will become important and relevant to the next generation of nanoelectronics devices and integrated circuits.

For instance, there will be a need to understand plasma-surface interactions in plasma synthesis, etching, and deposition of new materials and structures such as those that will be used in quantum computing, spintronics, high-power and high-voltage electronics, potential candidate technologies that may eventually replace CMOS, and novel memory architectures. Such materials may include but are not limited to carbon nanotubes, 2D materials such as graphene, h-BN, layered dichalcogenides (e.g., MoS_2), nitrogen-doped diamond, wide bandgap semiconductors such as gallium oxide for power electronics, ferromagnetic and antiferromagnetic materials, and ferroelectrics and multiferroics for low energy dissipation memory and logic and topological materials.

It will be important to address the role of plasmas and plasma-surface interactions in producing, processing, and patterning these materials. In addition, current limits to selective and uniform etching of these materials over large areas will need to be surpassed. While some technologies and knowledge will be transferrable from CMOS processing, new challenges specific to the new materials will arise and will need to be addressed. For instance, new plasma gas mixtures will need to be found for plasma etching; new precursors may need to be synthesized for their plasma synthesis (e.g., PEALD or PECVD); and interactions of these new chemicals and their fragments will need to be studied and understood. Some of the emerging materials, particularly metals in emerging memory and other technologies, are difficult to etch, and plasma gas formulations to etch them selectively and uniformly over large areas with high throughput do not yet exist and must be developed. In all cases, the plasma synergistically interacts with these gases and materials, modifying fundamental properties such as particle distribution functions and plasma potentials, that then affect the reactive fluxes onto these same materials. As the materials and gases become complex, the relationship between fundamental plasma and these materials becomes more complex, thereby needing advanced plasma control schemes.

As noted in PRO 1, even for materials used routinely in CMOS technologies, etching and deposition gases with high global warming potential will need to be replaced with alternative chemistries. Such chemistries need to be developed, requiring a deep understanding of plasma-gas and plasma–surface interactions in these plasmas maintained with new gases. In considering gases and plasma chemistries for etching or synthesizing emerging materials, the selection criteria should also include the global warming potential of the candidates. The new plasma chemistries should aim to utilize gases with low global warming potential and not emit gases with high global warming potential as a result of chemical transformations that occur in the plasma. If gases with high global warming potential cannot be avoided, their capture, abatement, and/or mitigation must be considered, best performed with plasma abatement techniques that are energy efficient.

6. Plasma processing of 2-D materials

2-D materials are so-called because of their large lateral dimension compared to their thickness, an important materials class with unique properties that may replace or expand the capabilities of CMOS technologies. Such materials are being explored, from candidates for single-photon emitters for quantum information processing networks to transistors for low-energy dissipation logic. While exfoliation and colloidal solution synthesis have been successfully used to make a variety of single electronic and optoelectronic devices based on 2-D materials on lab scales, fabricating networks of such devices on a large scale at relatively low temperatures will require a suite of plasma processes. These processes include plasma deposition, plasma etching and plasma surface treatment to synthesize, pattern and dope 2D materials. The low temperature of LTPs is a particular advantage for fabricating 2D devices on heat-sensitive substrates and within limited ‘thermal budgets.’ [13] There is a need to control the electronic and optical properties of 2D materials by controlling the stoichiometry of 2D compounds and introducing vacancies and local stoichiometry variations during their plasma deposition/synthesis or post-synthesis plasma treatments. Assembling devices and heterostructures for devices from 2-D materials will require their selective etching, layer by layer, over each other or masks, which in turn requires precise control of power deposition and transport in LTPs.

7. Plasma synthesis and deposition of micro- and nanoelectronics device components

Synthesizing microelectronic device components such as nanotubes, nanowires, nanocrystals, and quantum dots either in the plasma [14] or on a substrate surface and then interconnecting them to form a device network is an alternative to the CMOS paradigm of building devices layer by layer on the surface of a wafer. Individual nanocomponents can be used to make transistors, light emitters, and memory components. In principle, these components can be synthesized in the plasma and placed in precise locations or synthesized directly on the substrate surface. Nonequilibrium LTPs is a strategic synthesis technique for such components in high-purity and large quantities either in powder form or on surfaces, as demonstrated for a few materials such as silicon nanoparticles, carbon nanotubes, graphene, and 2-D materials such as MoS_2. The non-equilibrium environment in LTPs has several advantages for synthesizing nanostructures as nano-particle based powders which can then be put in the form of colloidal dispersions to be placed on substrates. The advantages include energetic surface reactions that selectively heat these nanostructures to temperatures that can significantly exceed the gas temperature, and so anneal the particles in situ, and in situ doping. Synthesizing high-quality defect-free materials in the gas phase at high temperatures and then placing them to form circuits or devices on heat-sensitive substrates opens new vistas for integrated circuit fabrication. These advanced processes using LTPs are one of a very small set of options that have the possibility of economically being scaled to high volume manufacturing (HVM).

Another advantage of a nonthermal LTP may lie in its ability to form metastable non-equilibrium phases of materials. These phases may form either due to the non-equilibrium environment the plasma provides or because the structures are stabilized because of their nanometer size, i.e., stabilizing the nanoscale structures that are not stable in bulk form. Embedding dopants into nanocrystals at high temperatures and quickly quenching them to produce hyper-doped materials may become possible in LTPs. Often, nanometer-size materials have unique properties not observed in their bulk form. For instance, silicon quantum dots (nanocrystals with diameters less than 4 nm) emit light very efficiently compared to bulk silicon and can enable optical circuits to be integrated with CMOS technologies. Fabrication of silicon quantum dots using LTPs has been demonstrated to be a controllable and efficient process, though scaling to HVM proportions remains a challenge.

However, in all of these examples, understanding and controlling interactions of LTP produced species with nanoparticles in the gas phase remains challenging. Nanostructures nucleate and grow in the plasma, becoming charged and act as part of the plasma – they become an additional charge-carrying plasma species. These nanostructures have high surface-to-volume ratios and, in some cases (e.g., single layer 2D materials), they are ‘all surface.’ Thus, during their synthesis, they present large surface areas to the plasma and strongly affect the plasma generation of species, charge distribution, and electric fields. Their properties are, in turn, determined by how their surfaces are affected by the plasma.

8. Understanding and controlling plasma-produced defects on surfaces and sub-surfaces

At the end of the day, the semiconductor industry thrives or suffers based on the *yield* of plasma processing of devices in chips. There may be a few hundred dies (or chips) fabricated on a single wafer, with tens-of-thousands of wafers processed a month in a fabrication facility. The *yield* is the fraction of chips produced from the wafer that work sufficiently well that they can be sold. A process will typically be introduced into manufacturing when the yield is at least a minimum value so that the process is profitable. (That minimum yield is typically a highly held trade secret.) Any improvement in plasma processes that then increases yield adds to the profit margin.

Defects play an important role in determining the material properties and device performance in integrated circuits, and so in determining the yield of processing. Defects can be beneficial and desirable or detrimental to device performance. They can be introduced intentionally by controlling the plasma produced activation energy and species delivered to the surface, or unintentionally by not having this control. Unintentionally introduced defects during plasma processing are also referred to as ‘damage’ as they degrade the device structures and performance, and reduce yield. For instance, intentional substitutional doping is routinely used to control materials' conductivity and electric fields at interfaces and may be beneficial. On the other hand, nanometer to micron size particles created in the plasma and eventually falling on the wafer surfaces are defects that reduce device yields. Thus, understanding the formation mechanisms of defects and controlling them through control of LTP plasma transport is vital.

Defects can be characterized as zero-dimensional (e.g., vacancies and substitutional impurity atoms), one-dimensional (e.g., dislocations), two-dimensional (surfaces and interfaces), and three-dimensional (e.g., inclusions and particles). Some defects may need to be controllably produced for a given application, while others should be minimized or eliminated. For example, dislocation-minimized diamond doped with nitrogen-vacancy (NV) defect centers represents a candidate for quantum computing or sensing as the spin states of this point defect present a two-level system that can be used for qubits. The NV center is a stable defect in diamond, comprising a substitutional nitrogen atom next to a carbon vacancy. Quantum grade diamond is grown by plasma enhanced chemical vapor deposition, and nitrogen vacancies can be introduced from nitrogen-containing plasmas, both requiring precise control of the reactive fluxed produced by the LTP. On the other hand, dislocations, which can destroy quantum coherence, must be eliminated, or their formation must be minimized. [15] In superconducting Josephson-junction-based qubits, LTPs are used to clean surfaces before metal deposition or oxidation, which is crucial for interface formation and affecting coherence times.

Low temperature plasmas are also used for patterning transmons (a type of superconducting charge qubit) especially when integrating qubits with CMOS manufacturing steps. Therefore, understanding defects that destroy quantum coherence and how they are produced in plasma processing is vital. Research opportunities also exist in controllably producing defects for use in scalable photonic quantum information processing networks. For instance, such networks require single photon emitters, which may be formed by plasma etching or treatment of 2-D materials (e.g., h-BN). [15]

The plasma-produced defects on the surface also affect etching and deposition rates. Defects may play important roles in etching and deposition mechanisms and are therefore important in atomic scale processing using PEALE and PEALD. It is important to understand (i) which species in the plasma produce defects, (ii) what kind of defects they produce, (iii) where the defects are produced, and (iv) how the answers to (ii) and (iii) depend on the plasma produced energies of the species in (i).

Metrology is needed to detect and quantify defects produced or healed when LTPs interact with materials and their surfaces, preferably in situ. Examples range from the atomic scale quantum coherence destroying defects in materials and interfaces in qubits to device-yield-reducing nanometer to micron size particles created during plasma etching and collapsed masks. This metrology does not currently exist. Detecting plasma-induced damage in plasma etching and deposition, preferably in situ, remains an important challenge. Equally important is avoiding damage or possibly reversing it by, for example, using precisely controlled plasma produced activation energy to anneal a dislocation or to selectively remove particle contamination.

9. Plasma chamber wall interactions

In a plasma processing chamber, many surfaces other than the wafer contact the plasma. These include the chamber walls, electrodes, materials surrounding the wafers, windows, dielectric used for coupling electromagnetic inductive fields to the plasma, and tubes and piping for pumping or bringing gases to the chamber. These surfaces contact either the active plasma or its afterglow (the decaying plasmas after a power pulse). Surface recombination of radicals and ions can strongly affect plasma species density.

Deposition on or modifying these surfaces with the plasma can change these recombination rates during the processing of a single wafer or from wafer to wafer, affecting process robustness and reproducibility. In PEALE and PEALD, the plasma modified recombination and reaction rates on surfaces can influence purge and cycle times.

There is a need to understand the interactions of plasma-generated radicals, ions, and photons on the chamber walls and how these interactions affect the concentration of various species in the plasma. There is a need for sensors that can be used in situ and in real-time to monitor the chemical and physical status of the chamber walls. The spatial constraints of the plasma equipment used in high volume manufacturing make the latter especially challenging. Opportunities exist for innovations for nonintrusive diagnostics and sensors with small footprints to determine the walls' state and monitor plasma-wall interactions in situ and in real-time. There is also a need for chamber wall materials or coatings that are robust and inert to minimize the influence of the walls on the plasma. Typically, in high volume manufacturing, chamber walls are cleaned or restored to a known state between the processing of each wafer to maintain wafer-to-wafer reproducibility. Although effective, this procedure can reduce throughput (wafers/hour) in a given plasma chamber. There is a need for more effective ways to manage the chamber walls as well as innovative new chamber wall materials and coatings that either reduce or eliminate the need for cleaning. Another possibility is to use real-time-control techniques to adjust plasma properties in response to the change in wall conditions to ensure that the plasma produced reactive species onto the wafer remain constant.

A related challenge is nonuniformities that arise at the edge of the wafers, where the surface material changes from silicon to another material. The concentration and electric field discontinuity at this location introduces nonuniform etching at the wafer edge, thus reducing device yields. There is a need to understand the nature of these nonuniformities and develop 'edge ring' materials that allow the control of electric fields and species flux gradients to eliminate the nonuniform etching.

10. Understanding material transport in plasma processing

In plasma etching and deposition processes, whether continuous or layer by layer (e.g., PEALD, PEALE), material from the wafer surface may be transported elsewhere in the chamber or vice versa. The former is how chamber walls become coated with etching products, and the latter may lead to device contamination and defects as atoms from various parts of the chamber end up in or on devices. Such transport can also be across the scale of features. For example, wafers are coated with numerous materials (e.g., masks, many device layers, etc.), and one material removed from one feature on the wafer may end up in another feature elsewhere on the wafer. Even in a single feature, especially those with high aspect ratio, etching and redeposition may lead to undesirable feature profile variations or contamination. In general, there is a need to understand how materials are transported between the surfaces in contact with plasma and control and eliminate such crosstalk between surfaces when needed.

11. Plasma-surface diagnostics

There has always been and will always be the need to monitor and quantify the chemical and physical state of surfaces in contact with plasma species with ever-increasing spatial and temporal resolution. These methods are collectively referred to as plasma-surface diagnostics. These diagnostics must be as nonintrusive as possible to characterize the surface without disturbing the surface or the plasma. In high volume manufacturing, it is difficult (and in some cases not possible) to directly have in-plasma diagnostics that monitor the state of the plasma. That said, characterizing surfaces in contact with the plasma and/or the plasma produced fluxes onto those surfaces is a sensitive measure of the state of the plasma. In situ plasma-surface diagnostics are preferred to collect information about the surface under processing conditions. This is a significant challenge because the existing arsenal of surface analysis tools relies on interrogating the surface with electrons, ions, and photons with well-defined energies under ultra-high vacuum (e.g., X-ray and ultraviolet (UV) photoelectron spectroscopies, Auger electron spectroscopy, secondary ion mass spectroscopy, etc.). Of the various particles, only photons with energies lower than UV can travel through the plasma with minimal interactions, limiting the diagnostics to photon-in-photon-out techniques. However, creative schemes, such as the spinning-wall technique [16, 17] have also been developed to employ UHV surface analytic tools, albeit to date for research reactors only.

There is a need to develop plasma-surface diagnostic methods and approaches to deploy a wider suite of surface analysis techniques to determine the species present on surfaces and their coverage, preferably in situ, and the plasma produced fluxes onto those surfaces. There is also a need to examine surfaces with surface analytic tools and probe microscopies after they have been exposed to the plasma environment without exposing the surfaces to air. In most cases, multiple surface diagnostics and gas phase diagnostics are needed to obtain a complete picture of the plasma-surface interactions.

In etching patterns or filling features on surfaces with thin films using plasmas, there is a need to monitor how patterns evolve during etching or deposition. Information such as the etched feature profiles or whether mask defects have developed are usually obtained post etching using scanning electron microscopy. There is a need to obtain this information in situ and in real time using optical or other methods. Such measurements would then enable real-time-control of plasma transport to produce the desired surface functionality. This may be an area where post etching SEM images may be used to train machine learning models to recognize optical signals from the surface and correlate them with feature profile shapes or mask defects, which in turn are outcomes of plasma produced fluxes onto the materials.

12. Physically based multiscale modeling and role of machine learning

As discussed in PRO 4, virtual models of plasma processes – sometimes referred to as 'digital twins' – are needed to speed up learning cycles and technology development. Theoretical modeling of the interactions of various species from the plasma with surfaces of the materials used in microelectronics and semiconductor manufacturing is challenging because the phenomena span multiple lengths and time scales from angstroms to meters and from femtoseconds to minutes, respectively. There is a continual need for physically based models ranging from fundamental principles (e.g., density functional theory - DFT) to molecular dynamics and kinetic Monte Carlo to those based on continuum material, momentum, and energy balances. Ideally, these are coupled hierarchically to yield reliable predictions or inform plasma equipment design and process development. Such models have evolved mostly in isolation.

For instance, DFT is used to examine individual reactions to calculate reaction energy barriers and reveals potential reaction mechanism pathways for plasma facing materials in plasma etching and deposition. Molecular dynamics uses force fields that may be derived empirically or from DFT calculations to extend this examination to the time domain. Continuum models are used to represent transport and reactions on the reactor scale. However, there is a need to combine all the approaches to develop models with ever-increasing complexity and accuracy and couple them with experiments to tune the unknown parameters (e.g., kinetic rate constants, etch yields, etc.)

With significant advances in machine learning and artificial intelligence, there is an opportunity to combine these approaches with physically based models or use them as tools to create virtual models. For instance, machine learning models can be trained with data created using physically based models or with experimental data or a combination, creating new vistas for combining experimental data and theoretical predictions. There is also a need to use the power of machine learning to harness more information from large data sets collected from plasma etching and deposition reactors and use this information to make forecasts about the status of the equipment, process, and components, and in turn control plasma properties to produce the desired materials modification.

13. Plasma-surface Interactions relevant to the reduction of greenhouse gases

Many gases used in plasma etching and deposition, as well as species formed by the plasma during processing, and which are emitted into the atmosphere as exhaust from plasma chambers, have large global warming potential (GWP). Fluorocarbons and hydrofluorocarbons have long been used with established, widely adopted processes in manufacturing. While abatement of the exhaust gases is current practice, there is a need to eliminate hydrofluorocarbon gases (HFC) from plasma processing to minimize environmental impact. This is a major challenge that has strong implications. The ability of plasma activated fluorocarbon gases to etch and form etch retarding layers on semiconductor, oxide, and nitride surfaces has long been exploited to tailor feature profiles and control selectivity. Finding gases or combinations of gases that can provide similar benefits and understanding how plasmas sustained in these gases interact with semiconductor, photoresist and dielectric surfaces remains a challenge.

2d. Potential Impacts

Advances and discoveries in understanding plasma-surface interactions will have both scientific and technological impacts. The research opportunities outlined above focused on low temperature plasma-surface interactions as they relate to microelectronics and semiconductor manufacturing. A fundamental understanding of plasma-surface interactions impacts other fields such as power generation via fusion, plasma use in medicine for wound healing and disinfection, and the emerging fields of plasma catalysis and plasma synthesis of chemicals.

Interactions of photons, electrons, ions, and radicals with material surfaces are commonly studied individually and in isolation, while their synergistic interactions are poorly understood for many plasma-materials combinations. Synergies are often encountered in plasma etching and deposition processes, which provides the context for studying these interactions. Scientifically, closing the knowledge gaps identified above will advance our understanding of fundamental processes that occur on material surfaces when combinations of LTP produced radicals, ions, electrons, and photons impinge on the surface.

Technologically, advances in improved understanding and control of plasma-surface interactions can enable integrated circuits, electronic, and optoelectronic devices to be built with atomic-scale precision, uniformly over wafer scales. Understanding plasma-surface interactions in the plasma-assisted synthesis and etching of quantum materials and generation mechanisms of defects can lead to qubits with increased coherence times.

PRO 3: Develop fundamental data and centralized databases to enable comprehensive low temperature plasma diagnostics and modeling

3a. Summary

In this PRO, data that is needed to understand the creation and concentration of reactive species in low temperature plasmas (LTPs) as well as data that describe the reaction kinetics of plasma-generated species on a solid surface are evaluated from the perspective of their availability and reliability for current and future needs in plasma processing of semiconductors. The term data here refers to quantifying fundamental interactions between atomic and molecular species in the gas phase, and with plasma produced species in the gas phase. These data include, but are not limited to, electron impact cross sections, products of electron impact dissociation of molecules, mobilities of ions, reaction rate coefficients for neutral and ion-molecule reactions, quenching coefficients of excited states, photon emission and absorption cross sections, energy and angle sputtering probabilities of energetic particles with surfaces, and reaction probabilities of neutral species with surfaces.

As noted in the preceding PROs, processing plasmas contain energetic electrons, a variety of positive and negative ions, and many chemically reactive neutral radicals. In addition, photons over a wide frequency spectrum are generated in these plasmas. Inter-species collisions play an important role in determining plasma dynamics. An accurate plasma model needs to account for the important collision processes between charged and neutral species, and with surfaces. Fundamental data for these collision processes is, therefore, central to developing accurate models of processing plasmas. A wide variety of gases and their mixtures are used for the etching, deposition, cleaning, and modification of thin films in the semiconductor industry. There are multiple methods through which fundamental data has been generated for these gases historically. For inter-species collision processes, data for collision cross-sections and rates as well as reaction products have generally come from atomic, molecular, and optical physics (AMO) experiments and theoretical studies. Except for a few brief periods, [18] focus of the AMO experiments has not generally been on gases of interest to the semiconductor industry. Therefore, the status of fundamental data for semiconductor industry relevant gases varies from fair to poor. Many new gases used for plasma processing have been introduced in the last 20 years due to increasingly stringent processing requirements. Little fundamental information about the underlying collision processes is available for these gases. It is impractical to characterize the status of fundamental data for all important gases. We therefore describe the major categories of inter-species collision fundamental data and focus attention on categories with the greatest fundamental data need.

As noted in PRO 2, plasma-surface interactions are of central importance to the semiconductor industry. Models of plasma-surface interactions rely on fundamental data characterizing underlying processes such as ion induced sputtering and reactive radical chemisorption. The accuracy of these models sensitively depends on the fidelity of the underlying fundamental data. For plasma-surface interactions, fundamental data has usually come from 'beam' experiments where specific processes of relatively simple species can be studied in isolation, molecular dynamic simulation with known interatomic potentials, or quantum chemistry computations. Some basic processes such as ion physical sputtering have been well studied historically [19] and there have been a few studies of processes such as reactive ion etching. However, little effort currently exists to generate fundamental information about plasma-surface interaction phenomena of importance to the semiconductor industry. The lack of reliable fundamental data is a major challenge in developing advanced plasma processes suitable to meet the needs of a rapidly growing and evolving industry, and in models for those processes.

New gases and materials are regularly introduced for plasma processing in the semiconductor industry, and it would not be practical to experimentally generate fundamental data for every possible gas and material combination. It is therefore important to develop quantitatively accurate computational tools that can be used to generate the relevant data, coupled with experimental facilities to thoroughly test prototype systems. In addition, it is important to have experimental plasma facilities where a suite of diagnostics capabilities can be used to thoroughly characterize some important classes of processing plasma systems.

This diagnostic data along with fundamental data can be used for modeling experiments and developing quantitatively accurate plasma models. Models should include validated mechanisms for plasma chemistry and associated plasma-surface interaction processes. Machine learning methodologies coupled with the experimental data can be used to develop and refine mechanisms in an efficient manner. These data should be made available in accordance with the FAIR (findable, accessible, interoperable, and reusable) guiding principles.

3b. Scientific Questions

Access to reliable and accurate data related to fundamental processes in the plasma and at surfaces is critical to future progress in plasma processing technology. Listed below are some of the important fundamental data related scientific questions and issues. These topics are discussed in detail in Sec. 3.c.

1. *How can cross-sections for electron-impact dissociation of molecules of interest for plasma processing application be rapidly measured or computed to enable fundamental understanding of plasma transport to reduce plasma process development time?*
2. *For electron impact dissociation, how can the dissociation pathways be determined in a reasonably quick manner with the goal being to understand the fundamentals of plasma-produced chemistry and so help reduce plasma process development time?*
3. *For electron impact collisions, what are suitable techniques to determine the energy and angular distribution of reaction byproducts? Are there approximation techniques for generating such fundamental data that can be used to enable quicker development of plasma chemistry mechanisms for plasma modeling?*
4. *How can plasma diagnostics be used to help generate fundamental data for electron impact collisions on molecules of interest for plasma processing applications?*
5. *How should reliable plasma chemistry mechanisms be developed and tested? What diagnostic techniques should be used for testing and refinement of these mechanisms?*
6. *How should data for fundamental processes governing plasma surface interaction be generated to enable fundamental understand relevant to leading-edge semiconductor manufacturing applications (e.g., atomic layer deposition and etch)? Can quantum chemistry and molecular dynamics models help in this effort, and can these models be made quantitatively accurate?*
7. *How can fundamental mechanisms for plasma-surface interactions relevant to important plasma processing applications be developed and tested? What experimental facilities are needed to facilitate development of accurate models of how plasmas modify thin films?*
8. *To increase the speed of learning and development of more accurate models, what metadata standards should be used to enable exchange of data sets and mechanisms?*
9. *What types of data are needed to accurately model plasma processes and plasma-surface interactions?*
10. *Can refinement and expansion of existing data & databases substantively expand the capability of existing diagnostics?*
11. *What infrastructure is needed to classify and prioritize the generation of data for LTP science and technology? Is there need of standardized plasma sources such as the GEC Reference Cell which can be deployed in multiple laboratories?*
12. *Is an open-source framework for database management and contributions needed having, for example, a well-defined application programming interfaces (API)? Should it be managed by a professional organization such as the National Institute of Standards and Technology (NIST)? How can it be managed so it becomes the primary source of reliable fundamental data for the plasma processing community?*

13. *How can machine learning enable faster development of reliable reaction mechanisms for plasma chemistry and plasma-surface interaction? What experimental data would be needed to help with this effort?*

3c. Scientific Challenges and Research Opportunities

In this section, the data availability and needs are assessed, paired with experimental diagnostics or theoretical approaches for generating them. Several critical data needs are highlighted, including electron impact cross-sections for new molecules (e.g., to replace high global warming potential (GWP) gases in current use), dissociation cross-sections for most molecular gases, ion-neutral collision cross-section for most ions, properties of solid surfaces interacting with the plasma, including energy and angular dependence of collision byproducts and most ions colliding with the surfaces, and relevant many-body collisions.

1. Data for plasma diagnostics and modeling

Energetic electrons play a major role in driving the chemistry in processing plasmas. To model these plasmas accurately, one of the major classes of fundamental data needed is the set of electron-impact collision cross-sections or reaction rates for the important ionization, excitation, attachment, dissociation, and elastic scattering processes, as illustrated in Fig. 3-1. Measurement and computation of these cross-sections was a major focus of the AMO research community in the past, although this activity has dwindled in recent years in large part due to lack of research support from Federal agencies. Multiple scientific journals, including reviews, are available describing the status of electron impact cross-section data for some important gases. For example, Christophorou and Olthoff thoroughly reviewed and evaluated available cross-sections for some of the major etching gases. [18] Cross-sections for some electron-impact collision processes such as ionization and dissociative ionization are relatively easier to measure or compute, so this data are more abundant and can often be computed with sufficient accuracy for new gases.

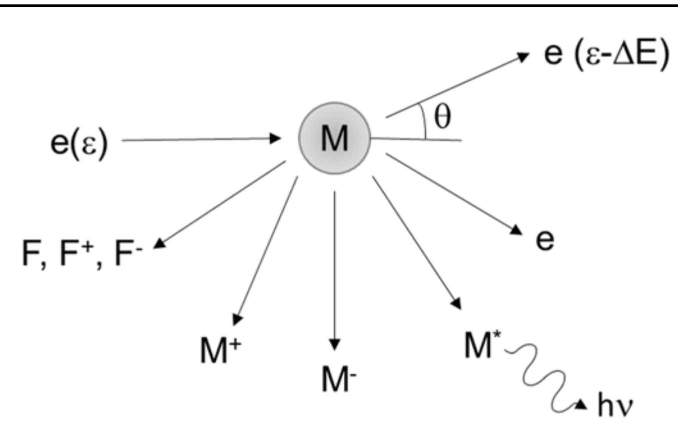


Figure 3-1: Schematic illustration of electron interactions with atoms and molecules

Among electron-molecule collision processes, one of the least studied yet most important is neutral dissociation. Neutral radicals play an important role in most plasma processing applications. Without accurate methods to determine which neutral radicals are present in these plasmas and the channels through which they can be generated and destroyed, developing quantitatively accurate models for plasmas of most molecular gases is difficult. In addition to fragmentation of the molecules into reactive radicals, these collisional processes are an efficient mechanism through which neutral radicals gain energy, a process that has been termed 'Franck-Condon' heating. Without knowing how energy electrons gain from the electric field is distributed among the neutral species produced by electron impact collisions, it is difficult to compute gas temperature in plasma models. Gas temperature determines neutral species concentration and so inaccurate gas temperatures result in quantitatively inaccurate plasma models.

A few techniques for measuring partial and total cross-sections for neutral dissociation are discussed in Christophorou and Olthoff. [18] There is a major need to refine these experimental techniques, apply them to some of the important molecules used in the semiconductor industry for etching and deposition, and test these cross-sections in plasma models. Direct measurements of dissociation cross-sections for O_2 and Cl_2 have only been made once, and only at energies far from the dissociation threshold, which is the most important energy range for the LTPs used in semiconductor processing. The contribution of electronically excited metastable states and of vibrationally excited molecules to dissociation is generally unknown. There is virtually no direct information about dissociation of fluorohydrocarbons with high GWP and for most gases used for current plasma enhanced CVD processes. Equally important as measuring electron-impact dissociation cross-sections is development of theoretical methods to rapidly determine the dissociation pathways and compute relevant electron impact cross-sections. Energetic electrons interact with molecules by perturbing the electron distribution in the molecule, creating electronically excited states. Much work has been done on this initial step, and methods based on the R-matrix approach are considered to be relatively mature. [20] These electronically excited molecules subsequently decay into various (neutral and ionic) fragments. Unfortunately, this second, crucial step is much more complex to treat theoretically, as it involves treating the motion of the nuclei in addition to that of the electrons. Convenient computational tools to predict the product yields, distributions, and energies are generally lacking. While it will be difficult to measure electron impact dissociation cross-sections for each molecule that is important for plasma processing applications, the experimental measurements can be used to test computational models for cross-section calculation for a (smaller) subset of the critical molecules.

Even when cross-sections for electron-impact processes are known, there is uncertainty about the energy and angular distribution of the reaction byproducts. For example, in kinetic simulations of processing plasmas, how the energy of the colliding energetic electron is distributed among the ionization byproducts and the angular distribution of the scattered electron can have major impacts on plasma properties. The properties of collision byproducts are currently guessed based on a few sparse measurements from the past, [21]. Producing these data needs to be elevated in priority.

As plasmas are typically quasi-neutral, ion transport properties influence not only the ion characteristics but the overall plasma dynamics. Fundamental data for ion-neutral collision processes are critically important to develop quantitatively accurate plasma models. In the past, swarm experiments were used to measure ion mobility and related ion transport properties. There are many excellent reviews and catalogues of this data. [22] However, ion transport properties were generally measured in collisional plasmas under conditions of DC electric fields, for generally non-reactive gases and for parent molecules (and rarely for ions of dissociation products). At low pressures when kinetic phenomena become important, cross-sections for ion-neutral collisions are needed. It is also important to understand the energy and angular distribution of the collision byproducts. These data are only available for a few simple gases. [23] Available theoretical models are often not applicable to complex molecules and to radical ion species. Without ion-neutral collision cross-sections, developing accurate kinetic model for LTPs sustained in molecular gases becomes a challenge.

Some of these data can be generated by exploiting various plasma diagnostics, including optical emission spectroscopy (OES), cavity ring-down spectroscopy (CRDS), laser-induced fluorescence (LIF), and two-photo absorption LIF (TALIF), combined with appropriate kinetics models to back-out the fundamental data. This process would be analogous to *unfolding swarm data* to produce momentum transfer cross sections and mobilities, perhaps now utilizing machine learning techniques. Optical and laser-based diagnostics offer the advantage of resolving temporal scales down to a few ns and spatial scales of a few micrometers, thereby allowing the measurement of plasma properties in the near vicinity of the wafer surface. [24]

OES: Optical emission spectroscopy is a useful diagnostic to measure densities, qualitatively and quantitatively, for a variety of atoms and small molecules. To quantify emission intensities and relate them to relative or absolute number densities, absolute calibration of the optical system is usually required. In absence of that calibration, rare gas actinometry is often used provide quantitative estimates of gas phase densities. Because of the complexity of the excitation process and energy mismatches, rare gas actinometry can only provide reliable number densities (relative or absolute) for a small number of cases. Requirements include but are not limited to cases where the emitting species is excited dominantly by direct electron impact of the ground state of the same species when quenching of the excited state is not important and when absorption of the emitted photon is small. Accurate cross section measurements are lacking for dissociative excitation processes. Cascading from higher excited states and radiation trapping can complicate the analysis. The emitting species also must have a threshold and relative energy dependence similar to the rare gas. The most common actinometer choice is emission from the $2p_1$ level of Ar, at 750.4 nm. The energy dependence of the electron impact excitation cross section for Ar $^1S_0 \rightarrow 2p_1$ is well known and appears to be a reasonable match to the relative electron impact excitation cross sections of several species of interest, including F, O and H atoms. This state has the advantage of not being excited to a significant degree from electron impact excitation of the Ar $1s_3$ and $1s_5$ metastable levels. While it is desirable to have the absolute cross sections for the species of interest, this is neither necessary nor sufficient.

OES actinometry calibration experiments can be conducted under plasma conditions, since number densities can be independently measured by optical absorption, LIF (laser induced fluorescence), TALIF (two-photon absorption laser induced fluorescence), or other direct methods. For example, calibrations have been carried out for F atoms to determine absolute reactive atom densities. Reliable actinometry calibration factors require testing under a range of plasma conditions that may produce variations in the electron energy distribution to demonstrate that little or no dependence of the calibration factors on conditions. Quantitative actinometry is most favorable for F, H, and N_2 with Ar, and Cl, Cl_2, and CO with Xe. Calibration factors have been published for these cases, while cross sections are also known for H, N_2, and CO. Due to the ease of use, especially in commercial tools where optical access is limited for many techniques, actinometry has a place in the diagnostics toolbox, and will benefit from additional calibration and cross section studies. That said, obtaining spatial information with any passive OES diagnostic is difficult.

CRDS: For cavity ring down spectroscopy (CRDS) measurements of atom densities, it is necessary to know the line strength (or Einstein A-factor) of the transition in question. For optically allowed transitions, the Einstein A-factors can be measured from the fluorescence lifetime of the upper state. However, this is not possible for forbidden transitions, because the emission is weak, and the lifetime is dominated by collisional quenching. In this case only calculated values are available. An example is the forbidden $^3P_2 \rightarrow {}^1D_1$ transition of O atoms at 630 nm used for the CRDS measurement of ground-state oxygen atom densities.

LIF: Laser induced fluorescence (LIF) enables the measurement of the relative densities of a subset of plasma produced radicals and ions, and measurements of ion velocity distribution functions. [25] Absolute calibration can be achieved by comparing the LIF signal to that from Rayleigh scattering from a known density of, for example, N_2 molecules. Unfortunately, many species which are important in plasma processing applications (e.g., BF_2^+, $C_xH_yF_z^+$, $C_xH_yF_z$, $SiO_xC_yF_z$, COF) lack excitation transitions at easily accessible wavelengths, or the excited states do not fluoresce (often the case for larger polyatomic radicals). Therefore, the data needed includes the identification of transitions suitable for LIF of species relevant to plasma processing, the transition strength (Einstein A coefficient), and the fluorescence yield.

TALIF: Absolute densities of certain atoms (e.g., H, N, O) can be obtained by comparing the TALIF (two-photon absorption laser induced fluorescence) signal using a nanosecond pulsed laser to that from a known density of a rare gas (Xe or Kr) that has similar excitation and fluorescence wavelengths. However, the accuracy is limited by the uncertainty of the two-photon absorption cross-section ratios, general only known to within a factor of two. At higher gas pressures, the effective lifetime of the emitting state must be measured to correct for collisional quenching of this state. At pressures approaching one atmosphere, the lifetime becomes so short that it is necessary to use picosecond or femtosecond lasers. These have the additional advantage that they favor multiphoton excitation of the probed atom over laser photolysis of the feedstock gas, which can otherwise cause overestimation of the atom density. However, there is a lack of reliable reference data for fs-TALIF. The fs pulse has a broad spectral envelope which can excite several transitions simultaneously in the calibration rare gas. A full quantum mechanical treatment of the excitation process becomes necessary for these short and highly intense pulses. It would be beneficial to build a set of references for plasma processing relevant species by performing fs-TALIF measurements on samples of atomic species with known densities (determined for example, by vacuum ultraviolet resonance absorption), under low pressure conditions, with no quenching, in order be able to tabulate the cross-sections for these transitions. Another important set of data is the natural lifetime for these elements, performed under collisionless conditions. While lifetime measurements for species such as Kr and Xe are well documented and accepted, measurements in H atoms, for example, have a large uncertainty due to a large spread in radiative lifetime values in the current literature.

Some of the additional fundamental data that are necessary to develop robust and predictive models for plasma processing systems include reaction (e.g., recombination) coefficients of neutral species on surfaces, coefficients of secondary electron emission due to energetic ion and electron bombardment on surfaces, electron recombination coefficient at surfaces, thermal accommodation coefficients of species at surfaces, rates for reactions involving heavy species (neutral radicals and molecules, positive and negative ions), and those of 3-body collisions (calculations from *ab initio* molecular orbital theory, group additivity method, *ab initio* transition states). Due to the wide variety of gases used in plasma processing, the variety of materials these species interact with, and the different conditions of these surfaces (i.e., surface coverages), fundamental data will not be available for every situation. Therefore, quick estimation methods or semi-analytic expressions for these fundamental data would enable progress on modeling complex systems.

The available data are currently scattered in the literature and there is often no critical assessment of the reliability of the available data. Some of these quantities, such as 'sticking coefficients' are undefined as they encompass multiple underlying fundamental processes at surfaces (including adsorption, desorption, reaction, recombination and deposition). Considering these uncertainties, plasma modelers often adjust these key parameters to match any available experimental measurements. A machine learning approach, coupled with measurements and computations, is likely to be a fruitful approach for determining rate parameters and mechanisms for plasma-surface interactions. Research should be directed towards more accurate measurements of fundamental parameters and developing rapidly executing models for computing them. At the same time, a systematic cataloging and critical review of available data are necessary. The NIST chemistry webbook is one source with relevant data for neutral reactions. However, this database is not geared towards the special needs of the plasma community; data are typically limited to reaction rates for neutral species and updates to the database are becoming less frequent.

There are independent self-funded or volunteer managed databases relevant to LTP modeling and diagnostics, perhaps the most successful being LXCat for electron impact cross sections and charged particle transport (https://us.lxcat.net/home/). LXCat is a community-wide, web-based project, involving researchers from more than 15 countries. Only a few datasets have reached the level of maturity such that they can be applied to a wide range of plasma conditions and reactors without additional verification and validation. Following the principle that "one size does not fit all", LXCat does not recommend data but provide tools to help users decide which data are most suitable for their application. There are also commercial offerings for data relevant to LTP modeling, one example being the Quantemol DB database (https://quantemoldb.com/). Assembling, verifying and distributing data sets with common formats are activities that can be community driven with participation by academia, national laboratories and industry. That said, data that are critical to the national economy and security, should be archived and distributed over the long term by Federal agencies. NIST and/or perhaps another government organization should play a role in data distribution and preservation by managing and maintaining these databases for plasma processing.

Equally important as data for individual physical and chemical processes are full plasma chemistry mechanisms with experimental validation, ideally utilizing multiple sets of experiments and from different groups. Currently, little effort is currently directed towards systematic refinement of plasma chemistry mechanisms for systems of interest to semiconductor processing, and very little work being funded in this area in the US. Much more progress is being made in developing reaction mechanisms for high pressure chemical conversion, and most of this work is being performed internationally (and in the EU in particular) due to lack of US funding in the area. Plasma modelers typically search the literature for available mechanisms and may find examples of plasma chemistry mechanisms for only simple gas mixtures. They must then decide how to extrapolate and extend the mechanism and data for the problem at hand. With enough adjustable parameters in these mechanisms, the modeler can often match available data. However, such models have limited ability to extrapolate beyond the conditions used for fitting the parameters. A systematic method to develop, rigorously test, and publish reliable plasma chemistry mechanisms relevant to semiconductor plasma processing is needed. Rigorous model testing and validation requires substantial experimental data sets, acquired under well-controlled conditions and comprising absolute density measurements of the key (stable and radical) species, measured over a range of gas pressure and plasma densities. An even more stringent test is for a model prediction to match time-resolved measurements in modulated plasmas. Such detailed data sets are rare, even for diatomic gases, since they are costly and time-consuming to perform. The GEC reference cell [26], developed in the late 1980s, was used for similar purposes with, in some cases, excellent results. A similar strategy is needed for current and future plasma processes.

2. Data for Diagnostics and Modeling of the Plasma-Surface Interaction

As discussed in PRO 2, understanding plasma interaction with materials, especially when the surfaces have nanoscale patterns, is critical to advancing the science of plasma processing in semiconductor device nanofabrication. Models for plasma-surface interactions range in scope from fundamental quantum chemistry-based techniques and molecular dynamics models to Monte Carlo based empirical models for feature scale evolution. The molecular dynamics and Monte Carlo based feature scale models rely on fundamental data regarding basic processes at the surface, and accuracy of these models is tied to the underlying data. The status of fundamental data for plasma-surface interactions is generally poor. It is currently not possible to conduct feature scale modeling without empirically selecting reaction probabilities by comparing or calibrating to experimental SEM (scanning electron microscopy) images of the features. The quantitative accuracy and range of validity of these models is therefore limited. Efforts should be directed towards developing quantitively accurate plasma-surface interaction mechanisms based on computationally generated data, experimental data, extensive experimental validation, and systematic refinement. A few leading-edge plasma processing applications such as high aspect ratio dielectric etching and plasma enhanced deposition of carbon could be used as prototype problems for systematic development and refinement of plasma-surface interaction mechanisms.

LTP interactions with surfaces is complex and a multitude of basic physical and chemical processes are responsible for the final structures on thin films. To accurately model plasma-surface modifications, the fluxes of ions, neutral radicals, and photons with these surfaces must first be known. Surfaces exposed to reactive plasma usually change dramatically from the original surface. An example is dielectric etch processes where ions and radicals are etching in the presence of a dynamic fluorocarbon film on the surface. The fluorocarbon film itself is formed by incident plasma produced radicals and ions, and atoms from the underlying materials being etched. Another example is deposition of dielectric films using plasma enhanced chemical vapor deposition (CVD). In these processes, neutral radicals and ions from the plasma react on the surface to form the growing film. The impacting, energetic ions have a significant influence on the growing film properties.

Plasma-surface interaction data exists for a few individual phenomena such as ion sputter yield on selected surfaces. [27] There are only a few plasma processing applications (e.g., metal deposition using physical vapor deposition (PVD)) where such data can be used directly. Even for ion sputtering yield, ion induced (and fast atom-induced) sputtering yield and its angular dependence, dependence on surface conditions (chemical composition and roughness) at energies of below 100 eV has not been reliably determined especially for advanced materials including modern ceramics, composite materials, nanomaterials, and thin films. Some of these data are derived from beam experiments dating from 20-30 years ago, where energy, angle and flux-controlled beams of reactive species successfully mimicked the halogen plasma-silicon surface interface. This success enabled the quantification of some key rate coefficients. However, such data related to chemical composition and surface roughness at energies of below 100 eV is not reliably determined for advanced materials including modern ceramics, composite materials, nanomaterials and/or thin films. To accurately characterize the chemical and physical effects of energetic ions, the energy and angular distributions of the ions must be determined.

Beam experiments were used until the 1990s to examine basic phenomena at surfaces in isolated conditions, as illustrated in Fig. 3-2. The fundamental data generated in these experiments continues to guide technology development. As semiconductor manufacturing technology has evolved, there is a great need to develop new measurement techniques for plasma-surface interactions designed to provide fundamental data for the state-of-the-art plasma conditions and materials. Emphasis should be on examining the etch, deposition, and film modification processes not just on planar films but within high-aspect ratio structures. Fundamental data generated in these experiments can guide the development of the plasma-surface interaction mechanisms discussed above. Some examples include ion energy analyzer (IEA), mass spectrometry (MS), spectroscopic ellipsometry (SE), and Fourier transform infrared spectroscopy (FTIR). These methods are summarized briefly.

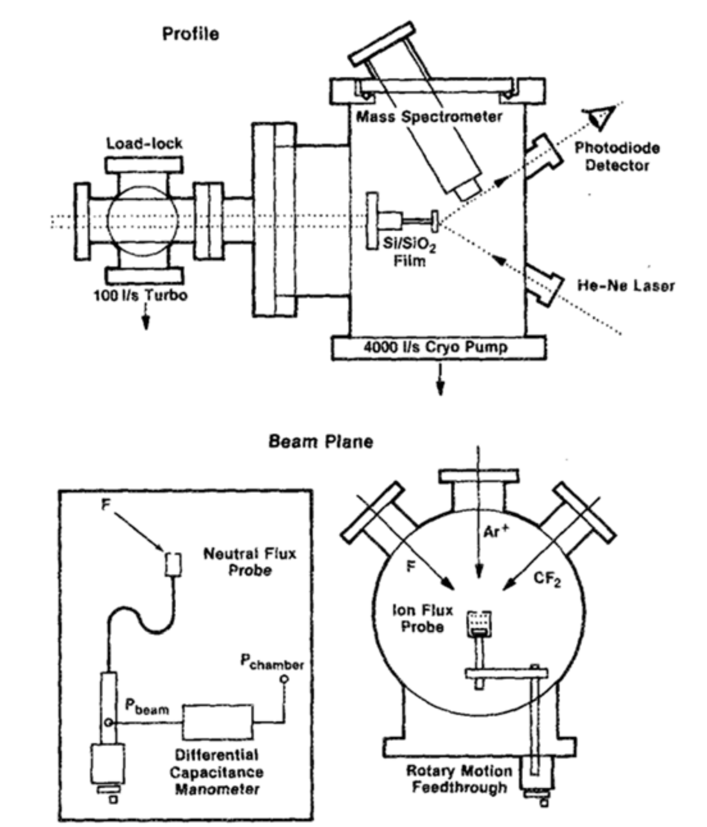


Figure 3-2: Experimental apparatus for beam experiments, simulating a plasma environment, while independently controlling the ion and neutral fluxes, their energies, and incident angle. Image from Ref [163].

IEA: Ion energy analyzer for measuring ion energy and angular distribution: Through collecting electrons and ions through gridded small apertures with various electric fields, ion energy and angular distributions as well as the mass of the ions can be determined. [28, 29, 30]

MS: Mass spectrometry (MS) for plasma species identification and quantification: MS can effectively measure and quantify positive and negative ions incident onto surfaces from the plasma. The ionic species from the plasma can be identified and directly measured by MS. To measure neutral species, either appearance potential MS can be used to distinguish neutral species by their ionization threshold, or direct cracking of the neutrals can be done at a fixed energy for analysis if the cracking pattern of parent molecules are known. Since reactive species exiting the plasma can collide with surfaces within the mass spectrometer before reaching the ionizer, live sampling generally requires at least two stages of differential pumping, line-of-sight detection through aligned apertures, and a chopper for phase sensitive detection. These constraints imply that measurements of fluxes to and from plasma-exposed substrate surfaces (as opposed to chamber walls) can be challenging.

SE: Spectroscopic ellipsometry (SE) for rate determination: SE is an accurate diagnostic to determine the thickness of a thin film. SE is nondestructive and can determine *in situ* thickness change, which defines the deposition or etch rate. As ellipsometry is sensitive to the optical constants of a material, it can be used to monitor deposition or etching, provided that the optical contrast between layers is sufficient. [31]

FTIR: Fourier transform Infrared spectroscopy (FTIR): FTIR, when combined with the use of an attenuated total internal reflection (ATR) crystal in contact with the plasma, provides in-situ and real time measurement of the composition and depth of thin films on surfaces. These measurements can be used to evaluate plasma-surface chemistry during deposition or etch processes. [32] Quantification of FTIR to yield absolute coverages requires absorption cross section data that are often absent.

Other diagnostic methods: While a variety of diagnostic methods are available to probe the condition and composition of surfaces in contact with LTPs (e.g., photoelectron and Auger electron spectroscopy, CARS, sum-frequency generation, second harmonic generation, glancing angle x-ray spectroscopy, etc.), many of these methods do not provide absolute, calibrated values. Working towards that goal of quantitative measurements of the composition of plasma-facing surfaces will require fundamental data. As generating this fundamental data is costly and time consuming, a consensus on the most important of such data would aid in prioritizing these efforts, perhaps achieved by a workshop on the topic.

When photons, ions and excited states of atoms and molecules strike surfaces, there is a probability that an electron is emitted from the surface, a process known as secondary electron emission (SEE). The rate of secondary emission is important to the electrical properties of LTPs and the generation of reactive species. The net charging of non-conductive surfaces in contact with the plasma and net current collected by conducting surfaces is in part determined by SEE, which in turn determines the plasma potential and power deposition. SEE from surfaces bounded by high voltage sheaths produces energetic beams of electrons that contribute to ionization and dissociation processes in the bulk plasma. There is need for fundamental data for SEE (electron-induced eSEE, [33] ion-induced iSEE, photoemission, excited state-induced, SEE by high energy atoms, molecules) of materials and films relevant to plasma processing. [34] The data should include the yield of SEE and its angular dependence as a function of the energy and angle of the incident particle, the electron spectrum of the emitted electrons, and dependence of these properties on the surface coverage and roughness. The eSEE and iSEE data for most conductive bulk materials for incident energies above 100 eV has been measured and reported in the literature. For lower energy primary electrons (less than 10 eV) and ions (less than 100 eV), the data for the SEE yield and especially for its angular dependence either does not exist or is less accurate. The data for the energy spectrum and angular dependence of secondary electrons are also limited, with there being scarce data for incident energies less than 100 eV. For these energies, the accuracy of the existing data for the eSEE and iSEE is thought to be poor. Less well known are data for poorly conducting materials and dielectric materials, especially materials exposed to and modified by the plasma and for energies of incident electrons below 100-200 eV. Charging, not well-defined chemical composition (after exposure to plasma and air etc.) are all challenges for measurements of SEE properties for such materials. For many new dielectric materials, coatings, and films, the SEE properties are essentially unknown. It is important to develop experimental capabilities to generate low energy (< 50 eV) ion beams for understanding atomic precision etch and deposition processes.

Some of these data related to plasma-surface interaction can be obtained from molecular dynamics (MD) models which rely on interatomic potentials to represent the fundamental interactions between plasma-based species and the surface. An example of MD modeling is shown in Fig. 3-3. The potentials for MD simulations have been developed for only a few systems of interest for plasma processing [35] and the existing ones have primarily been used in qualitative studies of energetic ion interaction with plasmas. The potentials are often obtained from material science studies where the potentials were developed and tested for low-energy phenomena. Little experimental validation and quantitative testing has been done using these potentials for plasma-based phenomena with energetic ions and chemically reactive neutral species. If these models are refined and made quantitatively accurate, they can be used to generate the fundamental data needed for feature scale models for plasma-surface interaction.

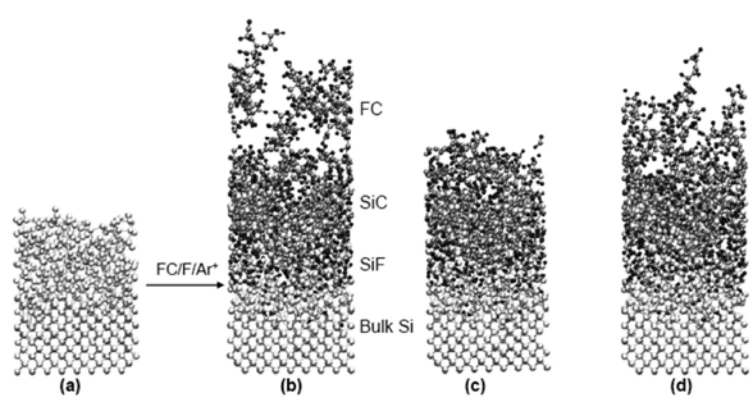


Figure 3-3: Molecular dynamics modeling results of fluorocarbon neutrals and argon ions, from Ref. [162]

There is significant

amount of fundamental data available in the literature and reports. However, it is generally too scattered and difficult for non-experts to judge which measurements or calculations are most trustworthy. This is where a reliable database such as the NIST chemistry webbook would help make plasma models more accurate, reproducible, and subject to continuous refinement. Attempts are being made in this direction in the plasma community, but they are either under-funded or in the commercial domain where data are only available to paid customers. An example of a publicly available database is the LXCat website [36] which includes data for electron and ion collision processes.

Quantemol-DB [20] is an example of a commercial database, which includes reaction rate coefficients and cross-sections for a variety of semiconductor industry relevant gases, as well as mechanisms summarized from the literature. Ideally, fundamental data should be hosted by a government agency (e.g., NIST) with oversight and review processes with strong participation from the research community. Periodic workshops would bring relevant people from different disciplines and communities (e.g., NIST, modelers, diagnostics experts, quantum chemistry and surface science experts, etc.) together to assess data needs and provide direction. The databases should ideally be publicly accessible with a well-defined application programming interface (API). These databases should be created in accordance with the FAIR (findable, accessible, interoperable, and reusable) guiding principles.

Generation of new fundamental data remains a perpetual need as new gases and materials continue to emerge, and the processing requirements continue to evolve. What is needed is (a) consistent efforts to develop accurate theoretical methods for examining fundamental processes in plasmas and related to plasma surface interaction, and (b) sufficient experimental effort to validate the modeling techniques. Theoretical models can then be used to generate quantitatively accurate data for new gases and materials. Facilities and capabilities of the following type are essential in developing and maintaining these needed data.

- Experimental facilities at which electron impact neutral dissociation cross-sections can be measured
- Experimental facilities at which energy and angle resolved data can be generated for the products resulting from ion and electron collision processes
- Theoretical models that can provide reasonable estimates of the neutral products of electron impact dissociation and their reaction rates
- Quantum chemistry-based models for moderate energy ion-surface interaction processes, especially in the presence of reactive radicals
- Experimental facilities where comprehensive diagnostic measurements can be done to test and develop plasma chemistry mechanisms and plasma-surface interaction mechanisms

Machine learning can be a valuable tool for developing mechanisms for plasma-surface interaction. How fluxes of various species from a low temperature plasma interact with a surface and generate products, whether at steady-state or in transients, is a fundamentally challenging problem. One could attempt to capture the overall transport and reaction phenomena by focusing on input/output (reactants and products) data and empirical/hybrid model generation, rather than on explicitly modeling the multitude of reaction/transport mechanisms. The issues that can be explored included:

- Capturing the functional effects of reactants on products by fitting data over a wide range. To develop a sensible approach, such data can be first generated using experiments, on which data-driven models can be fit, without explicit focus on fundamentals. The rich functional representation capabilities of tools developed in the machine learning field can serve the purpose. These machine learning models can then serve as the basis of feature scale simulations in relevant structures.
- A cycle of modeling/prediction/experiment/data can be followed, where data-driven models can suggest subsequent (computer or actual) experiments for maximum expected improvement of an objective, which, in turn, can generate more data and complete the cycle.
- The machine learning can also be used to develop and refine gas-phase mechanisms, by incorporating relevant and realistic physics/chemistry in describing these processes.

3d. Potential Impact

The availability of reliable and rapidly produced fundamental data will enable modeling and plasma diagnostics to investigate and better understand fundamental low temperature plasma properties, transport, plasma chemistry, and plasma-surface interactions. These models, diagnostics, and improved understanding will in turn support the development of novel plasma deposition and etching processes where complex material or heterostructures are needed with precise compositional control and conformality, as well as advanced plasma patterning process where reaction specificity, selectivity, and anisotropy are needed to achieve the integration of novel nano-electronics.

These reliable fundamental data and improved understanding of underlying plasma transport will enable plasma diagnostics and modeling to help mitigate the environmental impact of gases used in semiconductor manufacturing for deposition and etching. In the late 1990s, the mandate on limiting the use of perfluorocarbon gases (PFC) spurred concerted research activities that led to PFC reduction by a combination of process optimization, capture/recovery, and abatement. A recent mandate from the Environmental Protection Agency (EPA) based on the American Innovation and Manufacturing (AIM) Act requires the reduction, if not elimination, of hydrofluorocarbon gases (HFC), which are potent greenhouse gases. While the semiconductor industry has been working on reducing greenhouse gas emissions, PFC and HFC gases are still essential components for processing many materials and structures. With more and reliable fundamental data, it should be possible to identify plasma chemistries that are more benign, less hazardous, and more efficient in targeted deposition or etching processes. For example, the possibility of utilizing non-global-warming gases to create a plasma that mimics the chemical composition of PFC/HFC plasmas is appealing but is only feasible once reliable fundamental data is available to support these investigations.

PRO 4: Enable experimentally validated, predictive, and integrated modeling of fundamental low temperature plasma physics, chemistry, and surface interactions to enable next generation semiconductor plasma processing

4a. Summary

The plasma enabled fabrication of microelectronics devices is fully dependent on directly controlling the flux of reactive species to the wafer – charged particles, photons, and radicals. [37, 38] Those fluxes, and their energy and angular distributions (EADs), in turn determine the evolution of surface features which are the functional components of microelectronics devices. Those fluxes, and their EADs, are themselves dependent on the plasma processes occurring in the volume of the reactor, plasma-surface reactions occurring on the wafer and all surfaces in contact with the plasma, and the manner of power deposition (e.g., capacitively coupled, wave heated, dc magnetron). The assessment of power deposition and power coupling to the plasma depends on the matching of power supplies to the combined impedance of the reactor (including antenna, electrostatic chuck) and the impedance of the plasma itself. [39]

In order for modeling and simulation to have a meaningful impact on advancing the plasma enabled fabrication of microelectronics devices, these couplings and dependencies must be addressed and understood. At its very heart, this is a plasma chemistry modeling activity. At the end of the day, the relevant quantities that must be predicted are fluxes of reactive species (and their EADs) to the surface of the wafer and plasma facing surfaces. Underlying the ability to predict those fluxes is the need to properly represent the complex collisional transport of electrons, ions (positive and negative), neutrals and photons, and their coupling to the electric and magnetic fields responsible for power deposition. [40] A model that addresses, for example, collisionless plasma phenomena in rare gases may be providing keen insights to interesting plasma physics. However, to enable modeling and simulation to meaningfully impact the semiconductor industry, these models must predict reactive fluxes (and their EADs) to the wafer. [41] This is a requirement.

That said, modeling and simulation (M&S), and the validating experiments that accompany those models, must address what at first are two different perspectives and goals. The first is improving fundamental understanding of transport and reactivity in plasma and plasma-surface interactions through computer simulation. An important component of this goal is capturing that understanding in M&S tools that can be used for learning by professionals in the field. It is now true and will be true far into the future that a more foundational understanding of the underly plasma physics and chemistry on the part of professionals in the field will produce a better technology outcome. The second goal is to provide a design capable M&S platform that can be used to optimize the design of specific plasma equipment and processes. These capabilities must be able to address real design features such as the recommended gap between the edge of the wafer and the focus ring, and perhaps use as input the CAD files produced by commercial mechanical engineering applications. These must be physics-based design tools which address the most fundamental of low temperature plasma (LTP) phenomena. In meeting both goals, a robust and complete database of fundamental cross sections, reaction probabilities and transport coefficients are required (as described in PRO 3).

The semiconductor fabrication industry generally, and the plasma equipment suppliers in particular, have embraced plasma modeling and simulation, and that adoption has been impactful. The major chip manufacturers perform modeling to aid in process development and to help form the advice that they provide to the plasma equipment suppliers. The plasma equipment suppliers employ modeling to both help design and analyze the plasma tools, as well as to develop processes and recipes that are delivered with the tool. In large part, this modeling is now performed with commercially available software, open-source software, or software licensed from individual research groups at universities. Only a select few of the chip manufacturers and plasma equipment suppliers have developed (or are developing) their own codes, though this number is increasing. The greater and more widespread adoption and use of M&S in the plasma processing industry will be predicated on whether codes are solving the relevant problems, and that means predicting reactive fluxes (and their EADs) to the wafer.

Modeling and simulation are perhaps the capabilities that can most directly and most quickly be translated to industry in the form of university and national laboratory produced codes or as commercial software. The time between requests for updates and updated code to address a particular problem can be as short as days to a few weeks.

That said, the form in which the software is provided to industry is exceedingly important to its impact. The complexity of the plasma tools and processes, a situation that is not static and continually evolving, is continually pushing the capabilities of the available codes. Due to these dynamic needs, external support will be required for any software other than in-house developed codes. That support comes from the developers of the code, from an open-source community, or from the support teams of the suppliers of commercial codes. Any code translated to industry must have a support infrastructure to remain impactful over the long term. Code support for industry often requires exchange of proprietary information to, for example, address a particular set of operating conditions or geometry.

One of the advantages of in-house developed codes is that the support comes from within the company. Commercial software whose developers rapidly respond to requests, provide real-time support, and can protect proprietary information is a solution for users who do not have their own codes (or in addition to those codes). However, using commercial software also means that competitive advantage is the company's ability to use that software better than competitors, as opposed to using a better code. In-house developed software provides a competitive advantage but also requires significant and continued investment. Open source, national laboratory, and university software sits somewhere in-between. Open source codes can provide a robust distributed source of support from the user community but would likely not be able to address proprietary issues. Codes from individual groups in universities and national laboratories, with their ability to protect intellectual property through NDAs (non-disclosure agreements), can provide close-in support. However, long term support and alignment with their fundamentals-focused missions are issues.

The computing platforms on which the codes are executed, the ability to make code changes, and the speed of execution are also important considerations. At the time of writing this report, the majority of industrial plasma modelers use codes that execute on desktop level platforms or, at best, small clusters. Other than short term collaborations between national laboratories and universities, and companies, high performance computing (HPC) requiring remote access to thousands of processors is not now part of the semiconductor computing culture. This situation could be a consequence of the codes now commercially available or available from universities generally not being HPC codes, defined as requiring remote access to thousands of cores. This situation may also be partly a consequence of the currently available HPC codes not addressing the plasma chemistry needed for process design. This situation is undoubtedly also partly a consequence of intellectual property (IP) issues wherein designs of chambers, operating conditions, and recipes cannot leave corporate information technology (IT) systems.

Another component is the time required to achieve a solution. The computational problems now addressed in industry must have rapid turn-around times to be impactful. That said, the meaning of rapid turnaround is in the eye of the beholder. Requests from external customers must be addressed quickly (e.g., days). Computational tasks for designing equipment and processes have longer timescales. M&S platforms that require weeks of computation on tens of thousands of cores are likely not compatible with either of these scenarios. The ability to make code changes to address new problems also impacts this timeline. Developing software that is easily changed and validated is critical in this regard. This need-for-speed is particularly the case as machine learning (ML) becomes more widely adopted, and thousands of cases must be executed to provide a training set. If the use of HPC is to penetrate into industry, it must be in a manner that protects IP, facilitates rapid turn-around (including problem setup), addresses the needed plasma chemistry, is built around well-supported codes, and whose developers can react quickly to add capabilities.

4b. Key Scientific Questions

1. *What fundamental modeling and experimental validation capabilities, including new low temperature plasma diagnostics, are needed to enable predictive modeling of complex transient and multi-step plasma processing to reduce plasma process development time and complexity?*

Plasma equipment and process modeling have made hugely important contributions and impact to the development of plasma equipment and processes. [42] However, those contributions have largely been in a support role – helping to refine designs, understand processes and explain surprising behavior. These contributions have been generally and qualitatively predictive; and in some cases, quantitatively predictive. The goal of M&S is to simultaneously perform clean-sheet design of plasma equipment and processes. The advances that need to be made to meet this goal are in robustness and dimensionality; and expanding that envelope of quantitative predictability to a larger dynamic range of types of plasmas sources (e.g., inductively coupled plasmas (ICP), capacitively coupled plasmas (CCP), electron cyclotron resonance (ECR), microwave, magnetron), transient pulsed sources, very low bias frequencies (100 kHz and lower), very high source frequencies (100 MHz and higher), low pressure (< 1 mTorr physical vapor deposition (PVD)), high pressure (5-10 Torr remote sources), and beam sustained plasmas.

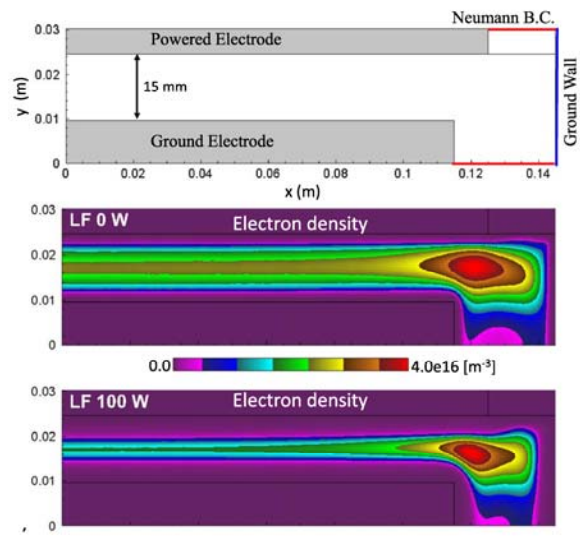


Figure 4-1: Particle in Cell (PIC) Simulations of Plasma Processing Reactors: Kinetic effects are important in charged and neutral particle transport in plasma etching reactors, as are 2- and 3-dimensional phenomena. PIC simulations are able to address such transport from first principles, providing the highest level of detail and accuracy. PIC simulations are challenged by heavy computational loads, and so are utilizing advanced computing architectures such as GPU (graphic processing units). The image shows the electron density from a PIC simulation using GPUs in a 2-frequency (13.56 MHz, 1.356 MHz) capacitively coupled plasma sustained in argon. A challenge for PIC simulations is to include complex plasma chemistry in 2- and 3-dimensions. [43]

To achieve the goal of 'clean sheet' design of complex plasma tools, 3-dimensional models executed on unstructured meshes may be necessary in many cases, though process optimization can likely be performed with more rapidly executed 2-dimensonal models. Arguably one of the goals of M&S is to reduce the complexity of current plasma tools. Over the large dynamic range of plasma tool operation that is currently in use, the transport of both charged and neutral particles will span from being local to non-local, with there being need to resolve energy (velocity) distributions in the bulk plasma and to surfaces. There are several computational techniques that can address this transport – purely kinetic (particle-based methods, such as particle-in-cell (PIC) [43] and continuum methods, such as direct numerical simulation (DNS)) and hybrid (combining kinetic and fluid techniques). [44] (See Figure 4-1.) As the pressure decreases, single fluid methods that are often used for neutral transport should be replaced with multi-fluid descriptions to account for the non-equilibrium in momentum and energy between species that can occur. For example, due to selective processes such as Franck-Condon heating following dissociative excitation or recombination, atoms can be significantly translationally hotter than molecules. At the lowest pressures, kinetic descriptions for neutral transport may also be necessary. This is particularly important for physical vapor deposition systems where sputtering of the target can produce neutral atoms having several to 10 eV of energy and mean free paths are large fractions of the chamber size.

Another form of non-local transport is radiation transport. As discussed in PRO 5, the consequences of visible, UV, and VUV radiation onto surfaces (wafer and chamber walls) are poorly understood. It is true that throughout the history of low temperature plasma materials processing, photon-stimulated processes have been occurring. However, with the exception of VUV induced damage of devices and low-k dielectrics, there has been little recognition of these processes. In developing next generation processes and plasma tools, M&S should also account for radiation transport and its effect on plasma properties (e.g., photoemission of electrons from surfaces producing energetic sheath accelerated electrons).

Developing models for LTP plasma transport to meet these requirements must also include the capability to address complex plasma chemistries. (See Figure 4-2.) There is certainly a place for more fundamental studies of basic plasma phenomena that may occur in plasma tools and those studies could be done with models that are not capable of addressing plasma chemistry. That said, the translation of those results to processing relevant conditions would be at best on a case-by-case basis. For example, in an ICP reactor, the spatial distribution of ionization sources and uniformity of the plasma is dramatically different between a pure argon plasma and an Ar/Cl_2=95/5 mixture. These processes are almost unrelated if comparing plasmas sustained in pure argon or pure Cl_2.

Another level of complexity that should be addressed in reactor scale LTP models, and by diagnostics, is the formation and transport of dust particles which contaminate wafers. [45] With killer-defect size of particles settling on wafers now only a few to 10 nm, even mild operating conditions can trigger the clustering and nucleation processes that result in formation of killer-defect particles. (A killer-defect renders a device inoperable.) The plasma chemical pathways for nucleation and growth of small particles are highly system specific, and poorly known even for the most common of chemistries. Although diagnostics are able to track large particles (hundreds of nm), tracking small numbers of 10 nm (or smaller) particles is at best challenging.

Also, as discussed below, the greatest impact that M&S will have on the industry is in utilizing the reactive fluxes produced at the reactor scale to predict evolution of features on the wafer. The requirements for these models are also discussed below. It is unclear what degree of coupling is required between the reactor and feature scale to enable model based, clean-sheet process development.

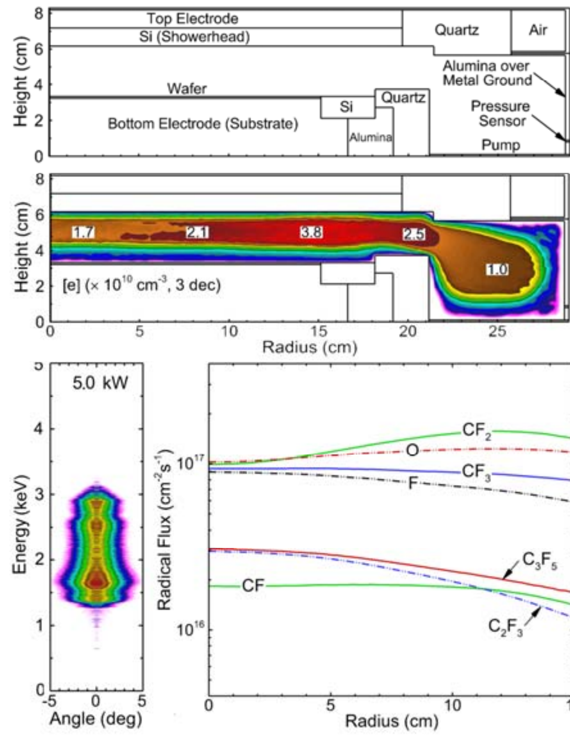


Figure 4-2: Plasma Chemistry Capable Models. Reactor and process design requires models capable of addressing complex chemistry in 2- and 3-dimensions, including material properties, multiple frequencies, and enough kinetics to predict particle energy and angular distributions (EADs) to the wafer (and plasma facing materials). The models must be capable of addressing long enough time scales to achieve a steady state, which is several gas residence times and pulsed periods. The image shows results from a hybrid simulation (combined fluid and kinetic techniques) for a 3-frequency (80MHz/10MHz/5MHz, 400W/2.5kW/ 5kW) capacitively coupled plasma sustained in $Ar/C_4F_8/O_2$ at 25 mTorr. The reaction mechanisms include 36 neutral species, 16 positive ions, 3 negative ions, and electrons. The cycle average electron density, EAD for all ions and neutral fluxes to the wafer are shown. [44]

To meet all of these requirements, a variety of computing platforms will be necessary. These computing platforms will span from desktop, global models to 3-dimensional, kinetic models executed remotely on HPC platforms. Before there is significant development on M&S platforms that are intended to meet industrial needs in support of semiconductor manufacturing, there should be discussions on how the models may be implemented.

All models should go through some manner of V&V – verification and validation. [46] Verification is the process to determine whether the equations in the model are being solved correctly. This can often be done using artificial (and sometimes non-physical) test problems. Validation is the process to determine if the physics in the model (transport algorithms, reaction mechanisms) properly represent experiments. Validation requires experimental data – and that requires diagnostics.

The range of diagnostics that are required to fully validate a model can be large. Ideally, measurements of the densities and temperatures of neutral and charged species throughout the reactor as a function of time are required. Values of electric field components and electric potential as a function of position of time, and electrical diagnostics (current, voltage, forward/reflected power) are also needed. The state of the surface, both on the wafer and on the reactor walls, must also be known as a function of time and position. The gas phase measurements will be provided by diagnostics including optical emission spectroscopy, absorption spectroscopy, laser induced fluorescence, E-FISH (electric field induced second harmonic), Raman spectroscopy, FTIR, mass spectroscopy, and electric probes (Langmuir, B-dot, capacitive) – and this is a non-exhaustive list. The surface measurements will be provided by diagnostics including ex situ XPS, attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR), scatterometry, photoluminescence, and interferometry. (See discussion on diagnostics in previous PROs.)

In past efforts to validate models, there has been little coordination between the modeling community and the diagnostics community. What can be measured is limited and the reactors in which the measurements can be performed are also limited. To some degree, diagnostics are made on species or quantities that can be measured for reasonable cost, which does not necessarily coincide with the values that are needed to validate a particular model. More coordination is clearly needed between the diagnostics community and the modeling community to determine what can be measured and what measurements are needed to validate the models. There will inevitably be a gap between these specifications. The community on both sides then work towards the center by developing new diagnostics and adapting models to use the diagnostics that are available.

A huge challenge in the application of models to plasma equipment design is the relevance of the validation. The plasma reactors developed for HVM (high volume manufacturing) have poor access for diagnostics. At best, there may be opportunity for optical emission spectroscopy or mass spectroscopy of the exhaust gases. In general, the more accessibility a reactor has for diagnostics, the less relevant the reactor is for HVM. There are certainly examples of HVM reactors being modified to provide optical and probe access. However, the on-the-factory-floor reactors typically do not have this access. The end result is that model validation will be done using diagnostics applied to plasma reactors that are, in some cases, geometrically and materially very different from HVM reactors, and with power delivery systems that are also very different. The challenge is then – how does validation of a model on these very different systems translate to process relevant HVM reactors? How far distant from a validated parameter space can the validation extend?

A second challenge is the availability of the diagnostics. A large set of diagnostics must be arrayed to fully characterize the plasma and surface processes. These diagnostics are likely not to be available all at one location. Reproducibility and relevancy of measurements made at one location to augment measurements at another location is and will be a continuing challenge.

One possible solution is development of affordable standard plasma reactors (akin to the Gaseous Electronics Conference Reference Cell – GECRC) that are geometrically and materially relevant to HVM reactors, while having the necessary optical and probe access. [47] These reactors would best be developed though collaboration of the diagnosticians, modelers, and industrial researchers. The reference reactors distributed to laboratories, along with standard operating practices, throughout the country (and arguably the world, as was the GECRC), enables measurements made in several locations, and simulations performed by many researchers, to be leveraged and combined into a comprehensive set for model validation. [48]

There are currently low temperature plasma (LTP) user facilities located at Sandia National Laboratories [49] and Princeton Plasma Physics Laboratory [50]. These user facilities have provided unique capabilities to the LTP community to make measurements in a variety of plasma systems, measurements that cannot be made at the investigator’s home institution. User facilities have and will continue to play a valuable role in providing diagnostics capabilities to the community. That said, it is likely not in the LTP community's best interest to focus all diagnostic capabilities in a small number of select locations. There is need for a broad approach to diagnostics, just as there is to modeling, to foster innovation, to provide hands-on experience and training for the next generation of scientists, and to enable long-term exploratory research. The final solution will be a mix of centralized diagnostics and distributed diagnostics. Where the tick-mark sits between the fully centralized approach and the fully distributed approach to diagnostics should be determined through a community consensus. If there was ever a need for a community workshop to make such decisions, this is the issue to have the workshop.

2. *What are the existing capability gaps in plasma diagnostics for advanced plasma processing manufacturing and how can they be closed using manufacturing-friendly sensor integration?*

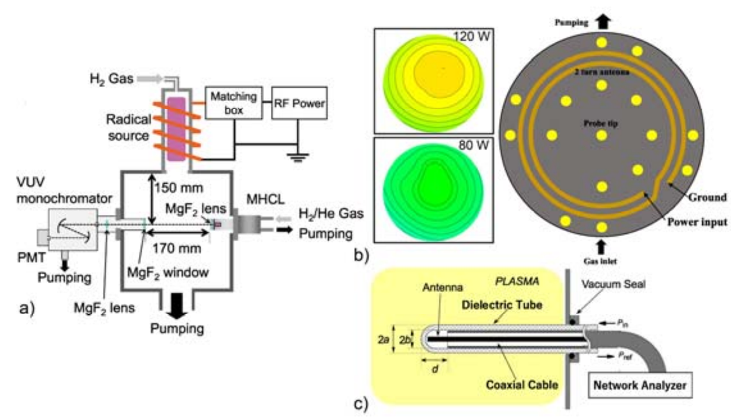


Figure 4-3: A comprehensive suite of diagnostics and sensors will be required to characterize the plasma and plasma-facing surfaces for model validation, real-time control, and equipment development. Measurements are required of electrical quantities (voltage, current, power), charged and neutral particle densities and fluxes to surfaces, temperatures (energy distributions) of neutral and charged species, and state-of-the-surface (etch or deposition rate, composition). Ideally, these diagnostics and sensors will be non-intrusive (not disturbing the plasma or surface), and spatially and time dependent. Examples of sensors shown in the images include: a) VUV absorption spectroscopy, b) on-wafer probes that measure spatially and time dependent fluxes to the surface, and c) microwave-resonance plasma density probes. A challenge in deploying these diagnostics and sensors is gaining access to HVM relevant plasma chambers for fundamental studies and model validation and employing such sensors in actual HVM equipment. [Images adapted from a) [51], b) [52], c) [53]]

Diagnostics of a plasma or plasma-facing surfaces requires access to the plasma or surface. Historically, plasma reactors used in HVM have poor diagnostic access, and so there are very limited direct measurements of plasma properties, and those diagnostics are totally non-intrusive. At best, the diagnostics may include current-voltage characteristics, mass spectroscopy of the exhaust gases, temperature measurements of plasma facing materials, and passive optical emission spectroscopy (OES). In many cases, the OES does not directly observe the plasma. Better diagnostics are required for real-time-control, endpoint detection, and actively managed processing. [51, 52, 53] To first order, better diagnostics require greater access to the active plasma and plasma-facing surfaces, and this access should be considered in design of new HVM plasma reactors. In the absence of greater access, non-intrusive diagnostics using the current access will need to be leveraged. These include higher fidelity optical emission or absorption, and face-mounted, in-wall probes. Such face-mounted, in wall electric probes are now available. The use of MEMS fabrication techniques for face-mounted probes (mass spectroscopy, ATR-FTIR) to sample the plasma or measure the state of the surface are other possibilities. The closer all diagnostics are to predicting the state of the wafer and the flux of reactive species onto the wafer, the more relevant the diagnostic becomes. (See Figure 4-3.)

As the aspect ratio and complexity of on-wafer features increases, endpoint detection becomes more difficult. (Endpoint is when the process has finished the desired goal; for example, etching through an overlying material to reach an underlying material.) Diagnostics are required that will precisely flag endpoint, using optical [54] or electrical means [55]. Current optical endpoint detection typically does not use full-spectrum data, and there are opportunities here to fingerprint processes using full spectrum data. The same can be said for diagnosing chamber conditioning.

Here again there are opportunities for machine learning (ML) approaches. [56] The difference between operation of HVM plasma reactors and developing new reactors and processes, is that the operating range of HVM reactors on the factory floor is limited. The plasma reactors on the factory floor typically run a repetitive process, that then enables accumulation of training data for ML. Large amounts of data from limited sets of diagnostics can then provide the training data for ML correlations that can be used to validate models. The validated models then provide the foundation for physics-based control strategies.

As in other areas, these activities cannot be performed in isolation. There is now a large gap between what can be measured in HVM reactors and what is ideally needed for real-time-control and model validation. A community-based discussion on how best to close this gap would be of benefit to all parties.

3. *Can plasma modeling be used to investigate new plasma reactor configurations and power formats? (e.g., magnetic fields, high frequencies, pulsed power, non-linear effects)*

The answer is clearly yes. Low temperature plasma models have already demonstrated their ability to investigate new configurations (reactor designs, antenna arrangements, materials, focus rings), power formats (frequencies, pulsed power, voltage-waveform-tailoring), magnetic fields (ECR, magnetically enhanced reactive ion etching (MERIE), magnetrons), and gas injection optimization (nozzles vs showerheads) while including the non-linear effects that occur from self-consistent coupling of physical processes (electrostatic, electromagnetic, kinetic). The outcomes of these modeling activities have had and are impacting the design of plasma equipment. These capabilities are now found, with varying degrees of dynamic range and type of plasma tool, in commercial software (e.g., COMSOL [57], Tech-X [58], CFD-Ace+ [59], PlasmaSolve [60], VizGlow [61], Plasimo [62]), university supplied software (e.g., HPEM [44], SOMAFOAM [48]), and software available from national laboratories [63], [64].

Given that the principle has been proven, what challenges must be met in order for model based or model enhanced plasma reactor design to become more impactful? In large part, these challenges are making the models more relevant to HVM processing conditions. Doing so means making plasma-physics focused codes more able to address complex plasma chemistries (10-15 ion species, including negative ions, 30-50 neutral species), surface reactions, advective neutral flow fields (gas injection and pumping), and radiation transport. These models must be able to address long enough time scales (many gas residence times and many pulse periods) to achieve a steady state, resolve transients, or achieve a pulse-periodic steady state. To be highly relevant to equipment design, these models should be able to accept CAD (computer aided design) files used to specify parts to define the geometry in the model.

4. *Can plasma modeling be used to investigate new process chemistries and predict their performance on a virtual platform?*

The answer again is clearly yes. LTP models have already demonstrated their ability to investigate new process chemistries. The challenges to make the capability more impactful are several. The most basic challenge is the availability of the fundamental data and reaction mechanisms for complex chemistries (see PRO 3). There is a history in process development to produce more complex chemistries, for example, gas mixtures with 4 or 5 components, most being complex molecules that are dissociated producing a myriad of dissociation products. In addition to requiring electron and ion impact cross sections for each feed gas, these data are also needed for each dissociation product, and the species that are outcomes of reactions between those dissociation products or with surfaces. A mechanism is then required for reactions between all of these species. Assuming the fundamental data exists (as discussed in PRO 3), the ensuing challenge is development of computational techniques that are robust enough to address this complexity. In the ideal, kinetic simulations should be extendable to dozens of charged particle species executed on unstructured meshes or structured meshes being able to resolve sheaths and equipment dimensions. Less capable models are still of extreme value when used in close collaboration with experimental plasma reactor development, to reduce the number of iterations required to finalize the chamber design.

A related challenge is whether LTP models can be used to reduce the current complexity found in process chemistries. This capability is particularly important in light of the required revamping of the majority of current recipes due to EPA regulation of the use of global warming gases.

5. *What modeling techniques are needed for in-feature engineering?*

Profile simulation is representing the evolution of surface features on the wafer (e.g., vias, trenches, atomic layer etching (ALE), deposition, fins) due to the reactive fluxes (ions, radicals, electrons, photons) onto the wafer from the plasma. [65, 66] From an industrial perspective, at the end of the day, this is the most relevant and final outcome of M&S. In order to perform accurate and predictive profile simulation, the reactor scale plasma processes must be understood and modeled. However, the final goal and outcome is profile simulation.

In profile simulation, material (atoms) is added (deposition or passivation) or removed (etching) from the surface, or bonds broken and created, in response to the incident fluxes. These processes include physical sputtering, chemical enhanced sputtering, thermal etching, adsorption, desorption, and photo-stimulated processes. These processes occur not only at the surface but also below the surface due to mixing by and implantation of energetic species. These processes also occur beyond the precise site at which, for example, an energetic ion arrives due to distribution of that incident energy. Nonlocal processes can also occur due to surface and through thin-film diffusion of physisorbed species.

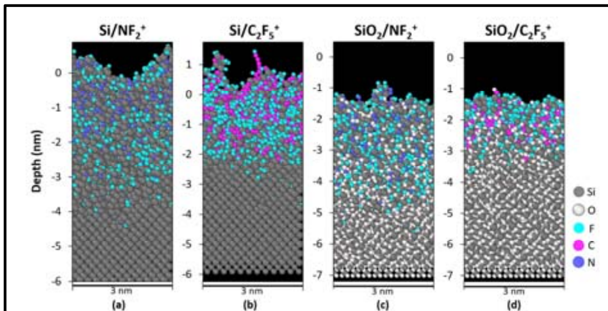
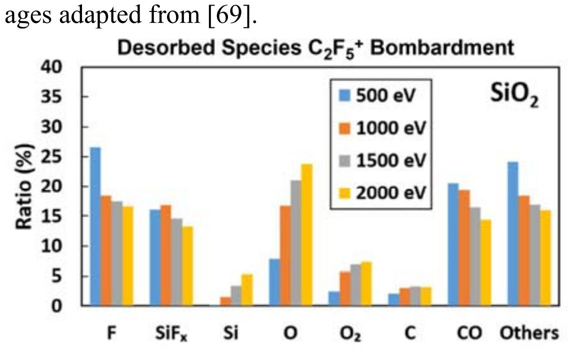


Figure 4-4: Fundamental Plasma-Surface Interactions by Molecular Dynamics. The interaction of plasma activated species and sheath accelerated ions with wafers (and plasma facing surfaces in the chamber) is at the heart of semiconductor fabrication. Molecular dynamics (MD) simulation is a first principles technique able to derive fundamental reaction probabilities and products, and predict the evolution of small features. The top image shows MD results for Si and SiO_2 after bombardment by 500 eV NF_2^+ and $C_2F_5^+$ ions. The bottom image shows the desorbed products following $C_2F_5^+$ bombardment of SiO_2. Although MD requires inter-atomic potentials between all atoms in the system, which typically comes from other quantum-mechanical techniques, it is one of the few techniques to quantify mixing, implantation and synergistic interactions. A challenge for MD is scaling to large enough spatial dimensions over long enough times to evaluate evolution of full features for complex materials. [Images adapted from [69].



The need for data and reactions mechanisms for profile simulation is perhaps even more critical than for the bulk plasma. A reaction outcome is required for every gas phase species arriving on every possible surface species, often as a function of incident energy and angle with respect to the surface. Reaction probabilities are also required for each surface species with every other surface species. These mechanisms apply not only to the materials forming the feature but also to the mask materials, as erosion of the mask and reflection of energetic particles from the mask are critical to the distribution of species deeper into the feature. Sputtered or etched species within a feature produce gas phase species which diffuse back out of the feature, and may redeposit on surfaces inside the feature and outside the feature – and reaction probabilities are needed for these processes

Electrical charging of features due to the disparity in the angular distributions of electrons and ions incident onto the feature is an exceedingly important process. Charging can lead to damage of devices and create electric fields inside features that deflect the trajectories of ions. These deflections lead to feature distortion such as twisting and notching.

An example of a state-of-the-art need in feature evolution is the simulation of multiple high aspect ratio (HAR) vias having aspect ratios of up to 100 with openings of tens of nm, through hundreds of alternating layers of SiO_2/Si_3N_4 with an amorphous carbon (or other hard-like) mask. The need to simulate multiple features results from charging inside one feature that produces electric fields in adjacent features. This charging and feature-to-feature coupling leads to pattern-dependent-distortion. (Pattern refers to the geometrical layout of features on the wafer.) [67] Another state-of-the art need in feature evolution is the HAR etching of gate-all-around (GAA) transistors composed of stacks or alternating layers of, for example, Si and SiGe. This process requires a combination of anisotropic and isotropic etching, with selectivity between two very similar materials.

Several modeling techniques are used in feature evolution – molecular dynamics (MD) [68], kinetic Monte Carlo (kMC) [66], and level-set methods (LSM) [65]. Each technique has its advantages and disadvantages. MD is the most fundamental approach and therefore potentially the most accurate. MD requires inter-atomic potentials between all possible pairs of atoms and nearest neighbors while also requiring very small timesteps (on the order of 1 fs). (See Figure 4-4.) MD has been very successful in addressing small patches of materials (a few to 20 nm square by 10-20 nm deep). [69] Addressing full HAR features (hundreds of nm to microns tall) or several finFET or GAA structures will be challenging. Models based on LSM are the most rapid and are able to address the largest features. However, these methods are intrinsically surface-focused, and so are challenged at addressing complex chemistry, non-local processes, and implantation. kMC is an expedient hybrid technique that retains the ability to address complex structures on the appropriate spatial scales while including nearly all of the needed processes. kMC is significantly faster than MD and significantly slower than LSM. kMC does not have the atomistic detail associated with MD and so its reaction probabilities and reaction mechanism must contain higher levels of approximation and tuning. A middle ground currently being employed for profile simulation uses MD and quantum chemistry (QC) calculations to provide fundamental data that are then incorporated into kMC and LSM simulations. More tightly integrating data generating MD and QC methods with feature scale capable kMC and LSM models would improve predictability.

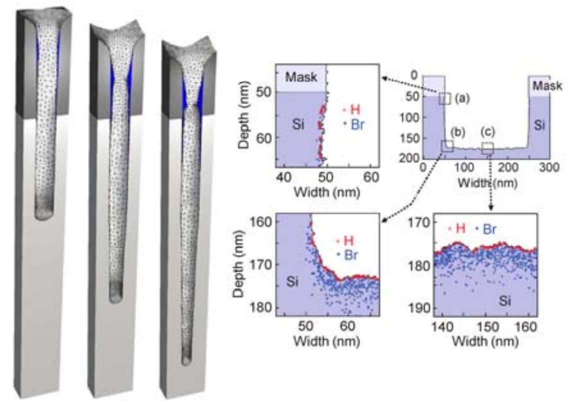


Figure 4-5: Profile Evolution. Perhaps the end product of M&S of plasma processing is prediction of the evolution of features in semiconductor wafers resulting from plasma produced reactive fluxes. Profile simulators use these fluxes and reaction mechanisms for physical sputtering, chemically enhanced sputtering, deposition, implantation, passivation, and surface diffusion to predict feature evolution on the nanoscale. There are two dominant profile evolution simulation methods. (left image) The level-set-method (LSM) is able to predict evolution of complex features using advanced computation methods. However, LSM is challenged by including first-principles surface chemistry, reactions between surface species, and implantation. This image shows evolution of a HAR etch in SiO_2. (right image) Voxel based kinetic Monte Carlo (kMC) methods are able to address complex chemistries, including surface diffusion and implantation, but are typically slower than LSM methods. The image shows implantation of Br into Si during plasma etching using HBr mixtures. The challenges for profile evolution include LSM including more complex chemistries and kMC methods increasing their computational efficiency; while both need to scale to larger spatial dimensions to evaluate pattern dependent processes. [Images were adapted from (left) [65] and (right) [66]]

6. *What are the best strategies for multi-scale modeling (feature to reactor scale)?*

The plasma reactor scale extends from tens of cm to about 1 meter for large chambers to perhaps tens of microns to hundreds of microns to resolve sheaths in high plasma density systems or small mechanical features (such as wafer-focus ring gaps). The feature scale extends from tens to hundreds of microns (to address layout issues within a single chip) to a few tenths of nm for ALE/ALD processes. (See Figure 4-5.) The nominal connection between the feature and reactor scale is in the fluxes of reactive species to and from the surface. Reactions on the surface change the composition of the surface that then changes surface reaction probabilities. The change in reactivity of gas phase species at the surface then changes the gas phase species densities. These couplings occur not only on the wafer surface but on all surfaces in contact with the plasma, leading to 'seasoning' of reactors (passivating surfaces to make them less reactive) and, in the extreme, erosion of materials (such as windows in ICP reactors and focus rings) that introduce sputter products into the gas phase.

The current state of the art is not able, in a single numerical mesh and single integration methodology, to bridge the sub-nm to 0.5 m dynamic range. (Recall that time steps scale with the spatial scale, requiring sub-ps timesteps on the feature scale.) The time to fully resolve a feature, such as a HAR etch, can be 30 minutes or more, which is well beyond the time required for a plasma to come into a quasi-steady state. Certainly, resolving more than a few features out of the many billions on a wafer would be extremely challenging in the fully coupled multi-scale model. To bridge these time and spatial scales, hybrid, time/spatial slicing, sub-cycling techniques will likely be needed. Intermediate approaches may be advisable. One intermediate approach is to use a surface chemistry model in the reactor scale model that has an equivalent reaction mechanism with respect to average sticking coefficients as would result from a fully resolved feature scale model. The surface chemistry model would execute far more rapidly while providing similar synergistic feedback to the plasma. Fluxes from the reactor scale would then be imported into the feature scale for more refined resolution of the surface processes.

7. *What is the role of machine learning in modeling next-generation plasma process and plasma source design?*

The role of machine learning (ML) in M&S for LTP enabled processing is perhaps one of the most uncertain of the many uses of ML in the semiconductor industry. There are at least four major roles for ML with respect to M&S: a) development of reaction mechanisms or reduced reaction mechanisms [70], b) (semi-)empirical models for real-time-control (RTC) [71], c) determining signatures for instabilities or unwanted plasma behavior [72], and d) process development [73]. By its very nature, ML methods are best applied to conditions which are repetitive or recurring. ML methods are valid over a limited parameter space for which the training data has been collected (and the algorithms trained). In this regard, the use of ML based control algorithms is an ideal application. In any properly operating plasma tool, the deviation from ideal conditions will be small, the recipes are generally fixed and the change in actuator settings required to correct observed deviations is small. A training set of data (either computational or experimental) can exhaustively cover the parameter space and need not be frequently regenerated (and algorithms retrained).

At the opposite extreme is ML based process development and feature evolution. This is the most challenging application of ML. The goal is to use ML to replicate behavior (e.g., change in taper of a feature as a function of power or gas mixture) of a training process, and then use the ML algorithms to speed the development of a different process. The difficulty is that there is no guarantee that the ML algorithms will transfer between processes (the training process and the new process). There is ample evidence that the algorithms will not, in general, transfer between processes. For those conditions, the algorithms need to be retrained for the new process, which then begs the question if you need to retrain the algorithms with each new process, why use ML if the experimental data are available? A more fundamental approach is required for process development which could certainly be augmented using ML. For example, physics-based ML holds the possibility of deriving fundamental, physics coefficients (e.g., reaction probabilities, cross sections) which, being fundamental, should better transfer to other processes.

The use of ML for model reduction is also a needed field of research which also should be addressed with care. One of the challenges of model reduction (ML or otherwise) is the breadth of application of the reduced model. The greater the reduction in, for example, the reaction mechanism, the narrower the parameter space that the reduced model will accurately apply. For real time control (RTC) where the operating space is well defined, model reduction will likely work very well. If the intent is to perform parametric studies of performance over a broader parameter space, the reduced models must apply to the entire parameter space.

8. *How can reduced first-principles models be developed for real-time control of plasma processes?*

The required completeness, robustness, and resolution of models varies by the intended application. M&S used for equipment design and development of new processes needs a high degree of robustness and completeness in order that all possible outcomes are accounted for. These models would likely need to be multidimensional, address complex plasma chemistry, resolve dynamics of oscillating electric fields, solve

Poisson's equation, account for radiation transport, and provide steady-state (or pulse-periodic) solutions. In principle, the entire operational parameters space is open for investigation.

The situation is different when using first-principles models for real-time control (RTC). Using a model for RTC would involve shadowing the physical process with a model that executes in parallel at the same time. Real time control is usually applied to stabilize a process or to keep a process on a prescribed path. If a diagnostic of the process detects a deviation from the desired path, the deviation is fed into the model, which then recommends a change in one or more operating parameters (e.g., power and pressure) to restore the system to the desired path. In this regard, the operational parameter space is fairly narrow, and the adjustments needed to operational parameters to keep the system on track or to remain stable should be fairly small. (If you need to make a factor of two change in a base operating parameter to keep a process stable, there is usually something terribly wrong and it is best to just stop the process.) As a result, the robustness and generality of a model for RTC can be significantly less than for plasma reactor or process design.

When coupled with the need for the models to execute rapidly (in real time) to shadow the process and respond to deviations rapidly (perhaps within a second), the complexity of the model should be limited. This may mean using global models, reduced reaction mechanisms, and theoretical expressions for nonlinear phenomena (e.g., beam-bulk instability) instead of direct computation. That said, there is no absolute requirement that the model must run locally using the computer on the plasma tool. In principle, the model could be run remotely on a large/fast computer with a stable connection to the plasma tool. There is a desire to not 'weigh down' the plasma tool with additional computations beyond essential features (e.g., sensors, wafer movement, actuators) and so remote (in-the-cloud) computations for RTC would both offload tasks from the tool while enabling more sophisticated models to be used.

4c. Scientific Challenges and Research Opportunities

1. Scale up from coupons to wafers

A typical procedure for developing a new plasma process is to use coupons (a small square of wafer) or to cover a wafer with a shield having a small opening exposing a small area of the wafer to the plasma. These small, exposed areas of wafers (coupons or open windows) are used to reduce the cost of creating test structures for developing new processes and reduce the cost of measuring outcomes. Once a process is developed using coupons, the process must be scaled to a full wafer. This scaling is difficult because an entire 300 mm diameter wafer interacts and affects the plasma differently than a small coupon. M&S could have a tremendous impact on assessing differences between coupon-vs-full wafer processing, and speed scaling.

2. Plasma Chemistry and Plasma Physics Complexity

Process relevant LTP modeling capable of predicting reactive fluxes to plasma facing surfaces (wafer and walls) must be able to include complex plasma chemistry, addressing continuity, momentum, and temperature (or their kinetic equivalents) of each species in 2- and ideally 3-dimensions, including radiation transport. Simulations must be able to achieve a (pulse periodic) steady state in a reasonable turn-around time. At the same time, fundamental plasma transport must be addressed to capture instabilities, non-local transport, and energy distributions of charged and neutral species. At present, achieving all of these requirements is beyond the state of the art. Plasma physics focused codes and plasma chemistry focused codes need to move towards each other to incorporate additional capabilities to meet these needs.

3. Accessibility and Speed – Reducing Complexity

To impact plasma equipment and process design, computational tools must be accessible to the industry and must execute fast enough to perform parametric studies and respond to customer requests, while respecting intellectual property. This may be an inconsistent goal while also addressing the needed complexity of multicomponent plasma gas mixtures. There is a role for reduced order models that capture the needed physics and chemistry while being able to address the accessibility and speed issues.

4. Process Capable Surface and Feature Profile Models

Surface chemistry models should become standard features of reactor scale plasma models. As the plasma chemistry in models becomes more complex, the need for surface chemistry models also increases, as these models provide the boundary conditions (flux from a surface as a function of flux into a surface) that then determine the properties of the plasma. Doing so then introduces multi-scale (time and space) integration issues, in addition to developing the proper plasma-surface reaction mechanisms. Feature profile modeling is perhaps at a crossroads. All current models capable of addressing full and multiple features use some level of approximation for reaction probabilities and processes such as implantation. Models capable of addressing those issues from first principles are not capable of full (and multiple feature) simulations. The first principles (but not process capable) models and the process capable (but not first principles) models need to work towards each other.

5. Non-invasive Diagnostics Suites and Accessibility

Developing non-invasive plasma and surface diagnostics capable of fully characterizing the plasma and plasma-facing surfaces, and providing data for model validation, is now incompatible with HVM capable plasma chambers which do not have the required access. We now have one set of diagnostics for plasma tool development and model validation, and a second set of sensors that are used for real-time-control (RTC) on HVM capable plasma chambers. This inevitably leads to a disconnect in translating improvements in fundamental understanding and implementing sophisticated controls schemes developed in university and national laboratories, and even in plasma equipment companies, to the factory-floor. This is another example of comprehensive (but not HVM relevant) diagnostics suites and the HVM relevant sensors (providing incomplete information) needing to work towards each other.

6. Need for Community Discussions

Many of these challenges will only be met through community discussions and workshops that bring together, for example, the diagnosticians and modelers. What can be measured today and what needs to be measured for model validation? How can this gap be reduced? What are the fundamental data requirements and how can they be met? What are the optimal modes of translating university and national laboratory produced modeling and diagnostics to industry?

7. Standard Plasma Chambers

Model validation and diagnostics development require a baseline of fundamental measurements and reference data that can be exchanged and collated. For the viability of the discipline, supporting intellectual diversity, and training of the next generation of researchers, these measurements should be made in laboratories across the domain, from the labs of individual investigators to central facilities. Standard plasma chambers would facilitate leveraging, comparing, and exchanging the resulting data. Following the success of the GEC Reference Cell in making the community more aware of how to replicate performance between reactors, these standard plasma chambers would have geometries and power systems relevant to HVM, while also having the needed access for diagnostics. A community driven effort in the form of a series of workshops, would best define the parameters of these standard chambers, the chemistries and operating conditions that would provide the baseline for code comparisons and validation, diagnostics development, and the procedures for modifying and adding to these specifications. A single standard reactor will not address all needs, and so a suite of standard reactors may be necessary. The suite has the added advantage of testing models and diagnostics over a larger dynamic range.

8. The Digital Twin

A goal in HVM plasma processing is that two nominally identical reactors running the same process will produce the same result. This is not always the case, and so matching performance of two or more plasma reactors or restoring the performance of a plasma reactor after maintenance is a continuing challenge. Is there a role for digital twins of plasma reactors, akin to the digital twins that shadow jet engines?

[74] The digital twin would be a comprehensive model of the plasma reactor that tracks the experiences and performance of the plasma tool, accounting for small changes in tolerances and materials, while recommending remedies to restore performance of the plasma tool or to predict when maintenance is needed.

4d. Potential Impacts

The deployment and widespread adoption of validated, comprehensive, and robust models for plasma reactor and plasma-surface feature scale processes, and real-time-control, for plasma enabled semiconductor fabrication will have industry changing impact. In today's mode of operation, M&S is typically in a support role, refining designs and providing insights to improve experience-based-design. M&S typically does not start the 'clean-sheet' design process. M&S should be starting the clean-sheet process. The need for M&S to lead in today's complex environment could not be greater. The situation in plasma aided semiconductor fabrication is very different than in aerospace and mechanical engineering where the clean-sheet design typically begins with computer simulation. This capability has resulted from decades of investment into computational fluid dynamics and modeling of solid mechanics, investments that have not been made into modeling of LTP reactors and plasma-surface interactions.

The need for M&S to open new paths to plasma equipment and process design could not be greater than it is today. Consider the challenge of narrowing the angular distribution of ions incident onto wafers for etching of high aspect ratio (HAR) features. The angle of the incident ion narrows with only the square root of the applied bias voltage creating the sheath above the wafer. Bias powers are now as large as 20 kW. Further narrowing the ion angular distribution by a factor of two following current practice would require 80 kW biases. Perhaps there are other paths towards achieving this goal that can be first vetted with M&S. The slowing of etch rates in HAR features due to ARDE (aspect ratio dependent etching) now demands longer than 30 minute etches. Doubling the aspect ratio without addressing ARDE, and following current practice, could produce 90 minutes etches. Instead, M&S based reactor and in-feature engineering could address the fundamental causes of ARDE, and so dramatically decrease process times while reducing equipment costs.

To support these needed advances in computations for the semiconductor industry, a new funding and collaborative model may be needed for the LTP community. A strength of the LTP computing community has been the diversity of approaches to problems by individual research groups that have produced the current software used by the industry. At the same time, the lack of robust, long-term, and perhaps coordinated funding of the LTP computing community has resulted in that community being less prepared to achieve the goal of whole device modeling, akin to that being sought in the fusion community for tokamak reactors through the Exascale Computing Project (ECP). The collaborative computing model in the fusion community has been enabled by funding levels far in excess of that for LTP computing. In developing this new funding and collaborative model for LTP modeling and simulation, it is essential to recognize the multidisciplinary nature of the whole device modeling challenge, a challenge that will not be met by only participation of plasma physicists.

PRO 5: Understand and control low temperature plasma generation of radiation, radiation transport, and materials interactions in semiconductor processing systems

This PRO is directed towards the role of low temperature plasma-generated radiation and is divided into two key challenges: 5A, for the generation and control of extreme ultraviolet (EUV) radiation for lithography; and 5B, for the role of radiation in plasma-assisted thin film etching, deposition, and surface processing in general.

PRO 5A: EUV radiation for lithography applications

5A.a. Summary

The continued quest and economic drive to extend *Moore's Law* is in large part dependent on photolithography to define the features that will be fabricated on semiconductor wafers. In photolithography, a radiation sensitive coating, called photoresist, is applied to the wafer. The photoresist is exposed to radiation through a mask which contains the pattern that will be transferred to the wafer. The radiation alters the exposed photoresist compared to the non-exposed photoresist. After this exposure, chemical processing removes the exposed photoresist (or the non-exposed photoresist depending on the process). This removal opens windows in the photoresist through which plasma produced reactive species will, for example, etch the wafer. Fabricating smaller and smaller features requires shorter and shorter wavelengths to expose the photoresist to make finer and finer patterns. *All industrially important photolithography has been performed with plasma-produced photon sources.* Beginning in the 1970s with features sizes of 5-10 μm, photolithography was performed with plasma lamps, with successively shorter wavelengths. In the 1990s to 2000s, the plasma lamps were replaced with plasma discharge excited excimer lasers, culminating in the ArF laser producing 193 nm photons, which were further compressed using liquid-immersion techniques. (See Figure 5A-1.) Sophisticated techniques are used to expose and define features on the wafer that are small fractions of the exposing wavelength, down to about 10-20 nm. However, there is a limit to this ability to define features smaller than the wavelength of the photolithography sources. Shorter wavelengths are eventually needed.

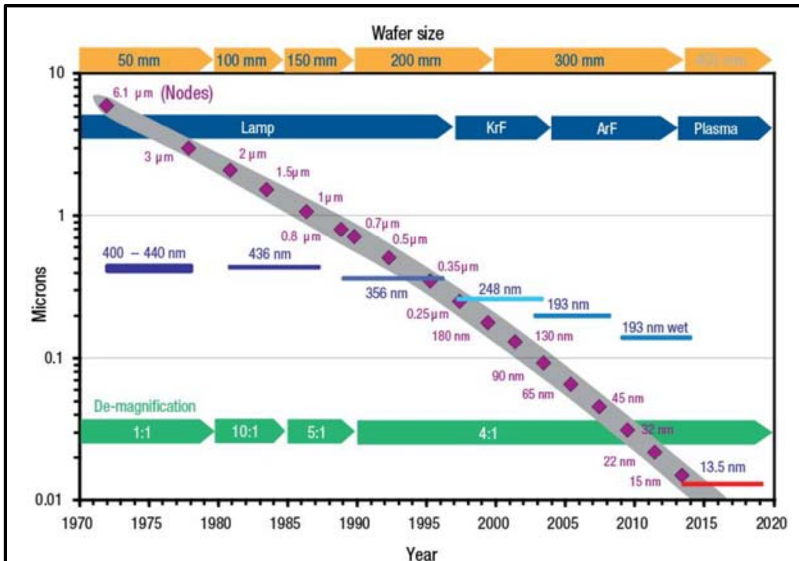


Figure 5A-1: Evolution of plasma based photon sources used to expose photoresist for photolithography in semiconductor fabrication. [172]

The current state of the art in photolithography photon sources is plasma generation of extreme ultraviolet (EUV) at 13.5 nm. [75, 76] EUV is capable of printing finer features in fewer exposures relative to the 193 nm photons produced by ArF excimer lasers, which can require up to four passes to expose the photoresist for one layer, a "multiple patterning" technique used to create smaller features than the wavelength. [77] The number of film etch and deposition steps is also reduced by the same proportion. This simplification also enabled 3-D patterning and additional innovations at smaller process nodes (e.g., < 7 nm). The 13.5 nm EUV photons have energies of ~92 eV. At this wavelength there are no transparent materials, so all optics must be reflective. The mirrors used must be Bragg or grazing incidence reflectors. For Bragg reflectors at near normal incidence, the wavelength is constrained by the selection of the multi-layer mirror materials and layer thicknesses and by the feasibility and efficiency of plasma emitters at those wavelengths. 13.5 nm was chosen such that Si and Mo bi-layers could serve as mirror materials. Highly ionized Xe, Sn, and Li are known to generate photons in this range. [78, 79] Several methods were investigated for the production of EUV photons at the power levels needed for lithography, including laser produced plasmas, discharge plasmas [80], and free-electron lasers [81]. Today, the only commercially available EUV photolithography system used in high volume manufacturing uses a laser produced plasma. A 10.6 μm laser focused onto a Sn droplet vaporizes and produces a highly ionized Sn vapor with plasma produced emission at 13.5 nm. [82, 83, 84]

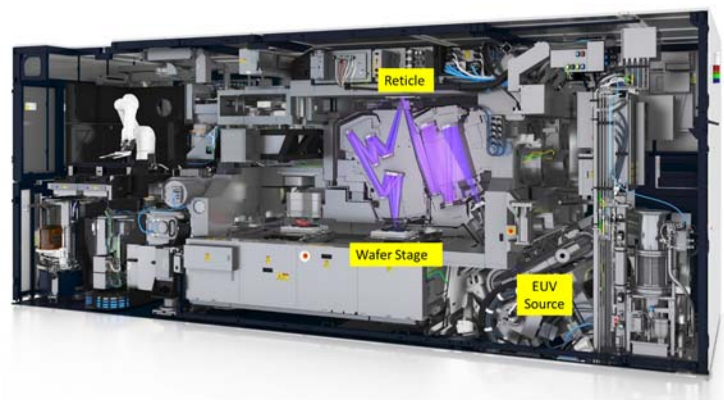


Figure 5A-2: ASML EUV scanner. The plasma source is in the bottom right of the figure and produces EUV (13.5 nm) light. The radiation enters the scanner and reflects off several multi-layer mirrors until it hits the reticle at the top of the figure. The reticle is a reflective mask containing the pattern to be printed on each field of the silicon wafer. Several more mirrors convey that pattern to the wafer at the bottom of the figure. A 300 mm wafer contains several hundred fields, and each field is scanned in less than a second. These machines scan over 100 wafers per hour with an accuracy of <1 nm in pattern overlay. (Picture courtesy of ASML.)

In current EUV sources, molten tin droplets with a diameter in the range of 20 to 30 microns are struck by a focused >20 kW CO_2 laser at a rate between 40 kHz and 100 kHz. [85] The laser light creates an intense plasma that ionizes the Sn to the +8 to +14 range where it emits in the UTA (unresolved transition array) band. [86, 87] Hydrogen is used as a background gas at pressures of 100 – 200 Pa because it has a relatively high transmittance for EUV photons, creating a secondary weak background plasma in the region irradiated by photons and ions from the primary Sn plasma. [88] A schematic diagram of a commercial EUV plasma is source is shown in Figure 5A-2 and the source is shown in Figure 5A-3.

This type of EUV source was introduced to high-volume manufacturing only at the end of 2019. [89] The plasma science associated with this source is therefore still in active development. Additional EUV plasma sources (so called "table-top") at a much lower average power scale are also a key area of development for metrology and for material and optical characterization. [90, 91, 92, 93] Advances in these metrology techniques are also needed to resolve structures during and after lithography with sub-nm precision, and in fundamental studies directed towards the improvement of masks,

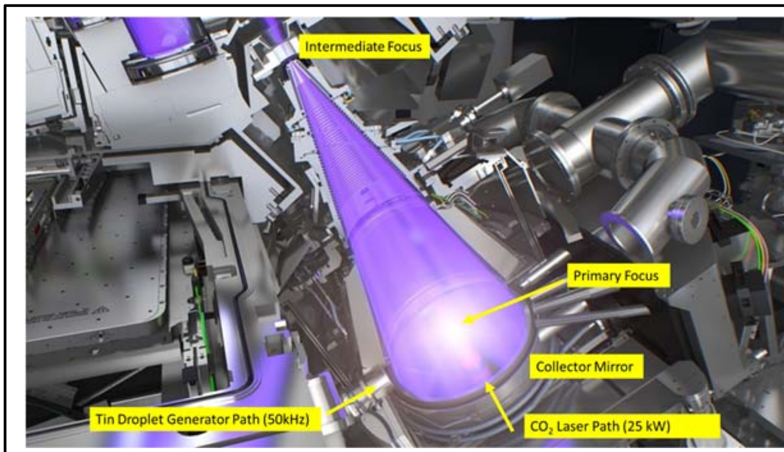


Figure 5A-3: EUV Source. Tin droplets are injected from the left at 50 kHz. They are hit by a pulsed 25kW CO_2 laser at the primary focus, creating an intense plasma. Light is emitted at a wide variety of wavelengths in all directions. The collector mirror is a multi-layer Bragg reflector with a spacing such that only light in the 13.5 +/- 0.2 nm band is reflected. That light is focused to the intermediate focus which is the entrance to the scanner. (Picture courtesy of ASML.)

pellicles, mirrors, and resists.

5A.b. Key Scientific Questions

The optimal path to create EUV photons capable of printing patterns on the order of the 13.5 nm wavelength on a semiconductor chip – the scale used at the "7 nm node" and beyond -- raises many questions and some of these are summarized below. Note that these general questions apply to any technology that can generate plasma capable of producing light in this energy range, but the laser-produced-plasma option will be used to illustrate the physics and engineering challenges.

1. Is there a more efficient plasma source to produce photons in the EUV range?

The EUV plasma produced photons required for lithography are generated via a cascade of processes, each with some efficiency penalty, giving rise to a few watts of EUV on the wafer for a ~1 MW wall-plug power consumption per photolithography system. [94, 95] Two of the most important components of this small system efficiency are the electrical wall-plug efficiency of the laser light needed for the laser produced plasma (typically on the order of a few percent up to ten percent), and the conversion efficiency of that laser energy into useful in-band EUV light emission (currently reported in a range between 2% and 5%, depending on the details of the target and wavelength). [96]

The CO_2 (gas mix CO_2:N_2:He) gas discharge lasers (10.6 μm) currently used to generate the laser pulses used for plasma EUV generation rely on a radio frequency (RF) generated plasma in order to generate the required vibrational state population inversion in the CO_2 molecule. [97] The wall-plug efficiency of the laser factors directly and significantly into the overall electrical efficiency of EUV lithography. The overall electrical-to-photon efficiency of the laser depends in part on maintaining the right balance of gas species in the plasma at the vibrational temperatures and densities to provide efficient gain for the laser pulse and provide a stable discharge. [98, 99, 100] Both the overall design of the laser flows and species collision rates as well as the detailed interactions of the laser plasma with the walls can have a significant impact on the wall-plug efficiency. Innovations in the laser plasma design and even in the choice of the laser itself could potentially deliver significant gains in efficiency, and reduced cost of ownership for chipmakers, leading to less expensive chips and higher production.

The conversion efficiency of the laser light into EUV radiation represents a second opportunity for overall efficiency improvement. For example, when focused laser light hits a molten Sn droplet, inverse Bremsstrahlung accelerates electrons causing rapid ionization. The material becomes 'warm dense matter' with an optimal plasma density on the order 10^{19} m^{-3} and an electron temperature in the range of ~30eV, at which the plasma's spectral emission is well matched to the passband of near normal incidence Bragg mirrors. At lower intensities, laser pulses can also be used to manipulate a spherical droplet's shape, for example creating a flattened nearly 1-D target that can subsequently be struck with a larger EUV-generating pulse. [101] While a more dense plasma may produce more EUV light, it will also re-absorb more within the core of the plasma, leading to an efficiency loss due to loss of the effective radiating volume. A lower density plasma will provide fewer radiators in the available etendue (spread in area and angle) of the collection optics for the EUV scanner. The engineering optimization of this balance over both the range of target sizes, morphologies, and densities over the time of laser pulse delivery constitutes the core design challenge in the efficient production of EUV light. There is significant room still for innovation and exploration in this area [102, 103, 104] that can lead to fundamental improvements to EUV production efficiency. The modeling of the plasma itself is a matter of considerable computational complexity, owing to both the highly dynamic nature of the radiation hydrodynamics, and to the complexity of the atomic processes participating in the EUV emission. [105] Advances in computational techniques targeting this regime can be expected to improve plasma engineering.

Current conversion efficiencies of the incident laser pulse energy to EUV photons are on the order of only 5% and this can likely be increased, as not all parameters relevant for the efficiency have been demonstrated to be optimal. It is also important to develop a more complete understanding of what happens to the remaining 95% of laser energy. Many other wavelengths of photons are produced, particularly in the

VUV range, which can themselves be transmitted to the scanner causing undesired effects, or contribute to undesired plasma chemistry in the gas or at surfaces. Further, fast electrons leave the plasma, accelerating ions in a 'Coulomb explosion' to many keV. These energetic hydrogen and tin ions would sputter adjacent surfaces, including the collector mirror, if it were not for the background hydrogen gas. [106] As the loss of EUV radiation to the gas is also a contributor to the total energy efficiency of the system, the optimization of ion energetics and ion stopping near the plasma becomes another key consideration for overall efficiency. [107]

2. *How do EUV photons and plasma species interact with the background gas, optical, and plasma facing surfaces in the EUV source and the lithographic scanner?*

The photon flux generated in the primary laser produced plasma in this pulsed process is large. Additionally, electrons, ions, and even the shock wave from the primary focus ionize the background gas and turn it into a plasma. This radiation and secondary plasma can interact with both the background gas and the optical and plasma facing surfaces, leading to complex, and in some cases, undesired effects. For example, the 92 eV photons impacting walls will emit photoelectrons with up to 70 to 80 eV. The re-emitted photoelectrons from the wall will have a distribution of energies, which can themselves generate plasma chemistry in the sheath region near the surface. This sudden electron flux from walls may invert the plasma sheath, thereby reducing the transport of ions or other particles. With multiple gas species present in the environment, there are generally multiple plasmas present. Their interaction and the resulting charge exchange processes can impact the transport of high energy ions from the plasma towards delicate optical surfaces, and can also impact the transmission and spectrum of the light from the plasma to optical surfaces throughout the lithographic system (scanner).

Within the lithographic scanner (also maintained in near vacuum hydrogen plasma environment), the plasma generated by radiation creates an aggressive environment which can reduce the overall optics lifetime in a number of ways, including roughening, blistering, chemical sputtering, and enhanced particle release. [108] In the area where a greater risk is from direct deposition of contamination (e.g., Sn) from the laser-produced plasma, the incidental or deliberate engineering of hydrogen radicals near the optics can actually deliver cleaning of the surface [109], aiding the overall optical transmission of the system over time. Demonstrating control over the plasma near the optics is a key consideration for engineering for EUV lithography. Improving optics lifetime can lower the cost of ownership and raise the productivity of the overall system.

There are several other plasma facing surfaces composed of a range of metallic materials in the region of the plasma. For the most part, it is not well understood how energetic species from the plasma affect wall materials and debris products (like solid or liquid tin). As current high-volume manufacturing targets lithography system availabilities (fractions of time operating) of >96%, the management of the plasma-radiation-wall physical chemistry is a key consideration for an industrial EUV source for lithography. Advances in the knowledge of cross-sections (both photon, electron, and collisional) and demonstration of control over the resulting plasma kinetics and transport processes near walls can aid the engineering of the plasma facing surfaces in such systems and significantly improve the cost of ownership and availability for the overall system.

3. *What happens to Sn in the plasma ablated droplet and how can it be managed?*

Specifically for the current EUV source architecture, the transport and control of Sn species following plasma ablation of the Sn droplet is of primary importance for maintaining the cleanliness of the EUV collecting mirror closest to the plasma. Much of the Sn which radiates to produce the EUV photons remains in the system and will coat mirrors and walls. A significant fraction of the Sn exits through pump ducts. Depending on the local temperature, this Sn can be either in liquid or solid phase. A Sn film of even 1 nm on a mirror will severely degrade its reflectivity and therefore the throughput of the scanner. [110] [111] The hydrogen gas used to slow the energetic particles has another function. Hydrogen radicals are produced by photodissociation from the EUV and by the plasma produced by the droplet expansion. The H radicals etch Sn to form stannane (SnH_4) which is volatile but reactive with adjacent surfaces. [112, 113] The kinetics of the formation of SnH4, and its resulting transport through the plasma environment, are complicated by the well-known thermal instability of the molecule. [114] The transport and chemistry of stannane with the materials and the background plasma is not well understood, but can lead to unexpected phenomena. An example from the plasma fusion community is in the formation of bubbles in liquid Sn under plasma loading, which can burst resulting in the undesired transport of liquid Sn debris. [115] Advances in the understanding of how Sn in liquid, solid, and gaseous (e.g., stannane and related molecules) forms interact and transport in a plasma environment will aid the engineering of EUV systems in the foreseeable future, owing to the central importance of Sn as an EUV emitter in the right band for lithography.

5A.c. Scientific Challenges and Research Opportunities

1. *Efficiently generate EUV light for lithography and for table-top metrology.*

It is likely that EUV light for lithography and for table-top metrology will continue to be produced by plasma induced emission. Competing methods for producing the desired spectra of and power levels for EUV radiation have not met expectations to date or are simply too expensive. Plasma based methods will likely dominate well into the future. For EUV production by laser produced plasmas, the optimal wavelength, target, geometry, and laser pulse shapes are not known. Advances in our fundamental understanding of laser-metal droplet-plasma interactions are needed to make assessments of spectra, efficiency, and final disposition of the debris in these systems. For discharge-produced plasmas, power scalable geometries that do not destroy electrodes are not now available. For table-top sources, the specific demands of the application may require a customized approach.

Investigating alternate methods of plasma-produced EUV are encouraged provided that the practical limitations and requirements of the method are taken into consideration. These new configurations should have a possible path of development that exceeds the performance and reduces the cost of the current state of the art. These new methods should also be compatible with locating the entire apparatus in a semiconductor fabrication facility. For example, an accelerator based technique for producing EUV that is 400 m long will not fit inside a fabrication facility at reasonable cost.

2. *Efficient, high repetition rate, high average power plasma excited lasers are needed for scaling goals of future processing needs.*

The current method of producing EUV for industrial lithography currently relies on a laser produced plasma. Using the same basic configuration, future higher productivity systems with projected etendue and conversion efficiency limits imply the need for pulsed lasers having the following characteristics: ~20 kW - 50 kW range at between 50 kHz and 200 kHz with 10 ns to 100 ns pulses with optimal wavelengths between 1 μm and 10 μm, with improved wall-plug efficiencies relative to current systems (~5% electricity-to-photon). The systems currently used for EUV production are plasma excited CO_2 lasers. Can these plasma excited laser systems be scaled to have the necessary specifications? Are other plasma-excited lasers scalable to these specifications?

3. *Identify and develop effective diagnostics and models for the multiple plasmas used in EUV production.*

There are three classes of plasma in the current process of industrial EUV production. 1) The primary EUV-producing Sn plasma, 2) secondary background plasmas sustained in hydrogen and wall-related gas species, and 3) plasma used to excite the laser. Improving EUV production for lithography will require new diagnostics and models to characterize and quantitatively predict the system performance of these plasmas over the lifetime of the system. For example, plasma diagnostics will help guide the development of higher efficiency EUV light production by identifying the intermediate species and transport phenomena which are at play.

5A.d. Potential Impacts

The potential impact of research in plasma sources for EUV production is nothing less than the ability to continue *Moore's Law* with the associated technological and societal implications. Although important advances in direct write technologies may be needed for future advances, photo-lithography with EUV and subtractive processing (etching) will dominate microelectronics manufacturing for the foreseeable future.

PRO 5B: Radiation in plasma etching and deposition applications

In any etching, deposition, cleaning or ion implantation plasma process, surfaces bounding the plasma, including the substrate, are exposed to fluxes of energetic positive ions, electrons, and reactive neutral species, as well as light generated in the plasma. In particular, high-energy photons can cause chemical reactions in chemisorbed layers on these surfaces, which can potentially lead to degradation of masking layers, insulating films, and critical regions of the silicon substrate. Large fluxes of UV and VUV photons can also lead to erosion of chamber materials. Nowhere are these concerns more important than in plasma etching. Anisotropic etching in plasmas is a critical means of pattern transfer into silicon, silicon dioxide, aluminum and other microelectronics materials. [37] It is well established that energetic positive ions accelerated through the plasma sheath at the surface of the wafer and impacting the surface at near normal incidence initiate or enhance chemical reactions. These ions also desorb products from the surface or inhibiting films in a layer of chemisorbed species (usually halogen-containing), leading to highly vertically directed etching of exposed areas through a photolithographically-defined mask. This positive ion-neutral synergy mechanism was first demonstrated by Coburn and Winters in 1979, [8] and has been confirmed for a variety of plasma-materials combinations. Energetic electrons can also stimulate etching [8], but electron bombardment with these relatively high energies does not normally occur in the type of low temperature plasmas (LTPs) used for semiconductor processing. Ion bombardment is also well known to cause damage to surfaces during etching and deposition processes. Photon irradiation, especially in the vacuum ultraviolet (VUV) region (<200 nm), is also thought to cause damage, though the mechanisms are less clear. Still less certain are the effects of VUV radiation on etching rates and feature profile shapes.

Since the initial use of LTPs for semiconductor processing, wafer surfaces have been illuminated by UV and VUV light. All processing recipes using plasmas have, by default, included radiation induced effects. With the exception of UV/VUV induced damage of semiconductor devices, there has been little acknowledgement of the influence of in situ, plasma produced radiation in plasma materials processing. That lack of acknowledgement also means that there have been no active attempts to control, enhance, or decrease the consequences of plasma produced radiation. This situation may have been a consequence of other processes needing more attention and control. However, the microelectronics fabrication process is now at the point where processes that result in monolayer differences in rates of removal (or addition) are critical.

5B.a. Summary

As critical components of integrated circuits proceed to ever thinner layers, low energy ion stimulated etching will be increasingly called for in applications where monolayer control and minimum substrate surface damage are essential. The etching yields (substrate atoms or molecules per incident ion) decrease at low ion energy. Hence the near surface region of substrates being etched are subjected to longer exposures to the plasma. This longer exposure can damage the etched surface, as well as lead to phenomena that could enhance etching and compete with the ion-enhanced process responsible for anisotropic etching. Among these, etching induced by VUV photons has been shown to be important in promoting etching of silicon in halogen-containing plasmas under some conditions. The complex interactions between plasmas and surfaces, especially semiconductor surfaces, are areas ripe for a deeper understanding that will benefit future plasma processing. VUV light also causes bond breakage in insulating and masking layers, leading to a loss of fidelity in pattern transfer during etching, as well as electrical damage that degrades device performance. UV/VUV illumination of surfaces can also produce secondary electron emission and desorb atoms, both leading to synergistic perturbation of the plasma.

The types of LTPs used in semiconductor etching processing produce light throughout the vacuum ultraviolet (VUV) to visible regions, as well as in the infrared (IR), spanning energies from typically ~20 eV to 0.1 eV. Light is produced by excitation of plasma species to emitting atomic and molecular states by electron-impact, excitation transfer and by dissociative recombination of molecular ions. Since the electron temperatures of most processing plasmas are between 1 and 5 eV, VUV light can only be produced by the small population of electrons in the high-energy tail of their energy distribution. For this region, the highest photon energies are limited to be not much larger than the ionization potential of the gas. VUV photon fluxes have been reported for Ar inductively-coupled plasmas (ICPs). [116, 117, 118, 119, 120, 121, 122] Values of fluxes striking surfaces range from 1×10^{15} to 1×10^{17} photons/cm^2-s, depending on reactor and detector geometries, power densities, and experimental uncertainties. These fluxes span about the same range as those for positive ion bombardment of the substrate. Plasma produced light, especially in the UV and VUV regions, can cause a number of effects during plasma-enhanced chemical vapor deposition or etching processes. While gas-phase photodissociation and photoionization are possible, they are likely small additions to the electron impact processes due to the relatively low photoionization cross sections in the gas phase compared to electron impact cross sections and lower densities of excited states that can be photoionized. That said, surfaces exposed to a plasma will absorb most if not all of the light escaping the plasma and striking that surface. Higher energy photons impinging on substrates can enhance etching, [9, 123, 124, 125, 126, 127] as well as cause damage that is often sensed by a degradation of a particular device electrical characteristic. [128, 129, 130, 131]

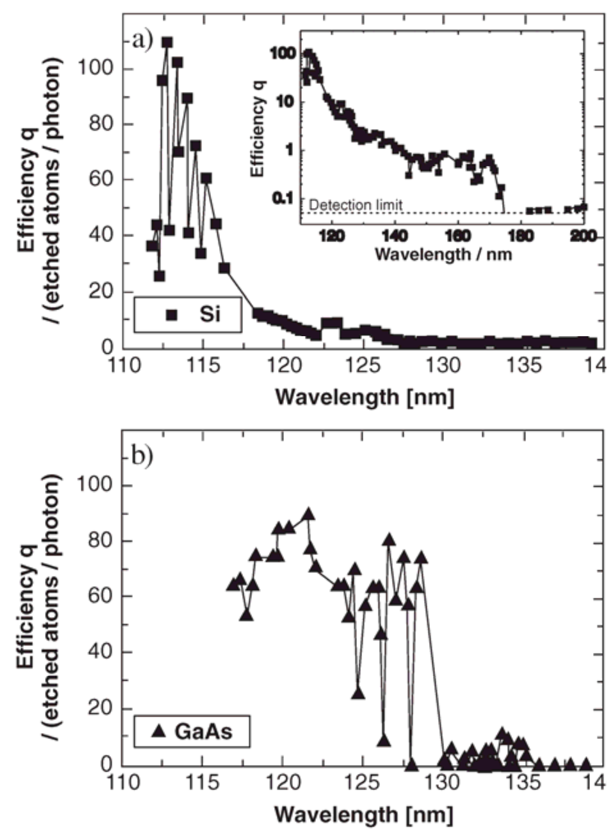


Figure 5B-1: Etching quantum efficiency as a function of synchrotron radiation wavelength for a) etching of Si(100) in the presence of XeF_2 gas and b) etching of GaAs in the presence of Cl_2 gas. [140]

Most studies of photon-induced etching of semiconductor materials have been carried out in a halogen gas atmosphere in the *absence of plasma*. [132, 133, 134, 135, 136, 137, 138] Though IR light has been reported to enhance anisotropic etching of copper in the presence of chlorine, [139] the majority of attention has been on the role of light in the visible to VUV regions. Semi-insulating and *p*-type Si (100) are etched if exposed to simultaneous Cl atom impingement (produced by photodissociation of Cl_2) and surface irradiation with UV or visible light. Etching is usually attributed to photo-generated carriers, though photodesorption has also been proposed as an explanation. In all of these studies, using light from lasers and lamps at wavelengths of ≥248 nm, the etching yields (Si atoms-per-incident photon) were much less than unity.

Schwentner and co-workers investigated photo-assisted etching Si in the presence of XeF_2 vapors, as well as GaAs with Cl_2, using shorter wavelength light produced by a synchrotron. [140, 141] In both cases, the number of Si atoms etched per photon dramatically increased below about 130 nm, and reached an incredible ~100 between 130 nm and 110 nm, as shown in Figure 5B-1. Furthermore, they argued that since most photons penetrated more deeply, the efficiency per absorbed photon at the surface was of the order of 10^5 Si atoms per photon. Such yields far in excess of unity were attributed to unspecified chain reactions. Yields higher than unity were also reported for Cu etching in presence of Cl_2 gas. [142]

Since such short wavelength photons are produced in the plasma, it is perhaps not surprising that similar, large photoetching yields of 90 to 240 Si/photon were recently found in plasma etching of p-Si(100) in a Cl_2/Ar ICP. [126] Photo-assisted etching of Si requires the presence of Cl atoms; no etching occurs with VUV light in the presence of Cl_2 gas. [126] Etched surfaces are smooth with insignificant undercutting of the mask (Figure 5B-2). The sidewall is sloped at an angle of 125° indicative of the (111) plane. Photoassisted etching of Si was also found in pure Cl_2 plasmas, as well as in HBr/Ar and Br_2/Ar plasmas. [127]

Though less reported on, photon-induced damage during plasma-enhanced chemical vapor deposition is also a continuing concern. VUV photons can create trapped charge or color centers, leading to a degradation in device electrical characteristics. This light can penetrate typically a few nanometers into films and can cause damage through thicker layers that are grown by a plasma-assisted process. It is difficult to tease out the effect of just the high energy photons when the substrate is also exposed to energetic ions, high-energy metastable atoms and molecules, and electrons. Hence carefully designed experiments are needed to isolate the photon effects.

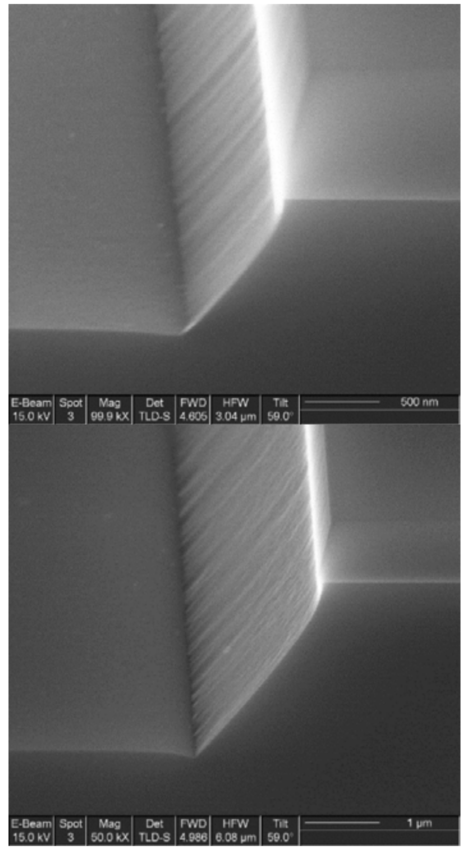


Figure 5B-2: Cross-sectional scanning electron micrographs of SiO_2-masked p-Si(100) in an Ar/Cl_2 ICP with added VUV light provided by an Ar ICP. Etching periods: top) 10 min, bottom) 30 min. [126]

5B.b. Key Scientific Questions

The potential impacts of VUV-induced effects on future semiconductor device development are enormous. For example, in etching of silicon (and other materials), the flux of VUV photons and energetic positive ions to surfaces can be comparable under some conditions, and the yields of silicon atoms etched per photon can exceed those for low-energy ions by a factor of 100 or more, while inducing undesirable etch profiles. These effects must be understood, controlled, and suppressed if the industry is to advance. Photoelectron emission from surfaces feed back to the plasma through changing the potential boundary condition and producing ionization and excited states by sheath accelerated secondary electrons. Some key scientific questions that need to be answered are listed below.

1. *How can UV/VUV photons generated in LTPs for semiconductor processing be controlled, customized, and manipulated to enhance (or de-emphasize) photon stimulated surface processes?*

The development of LTPs for semiconductor processing has been highly focused on controlling the fluxes of neutral radicals, electrons, and ions onto the wafer. There has been little, if any, emphasis on controlling the plasma produced UV/VUV photon fluxes onto wafers (and other plasma facing materials). Separately controlling, for example, ion fluxes and photon fluxes onto the wafer will be challenging. For example, increasing (or decreasing) power to increase (or decrease) ion fluxes will likely have the same effect on photon fluxes as the same electron impact processes that produce ions also produce UV/VUV photons. Increasing ion fluxes while reducing UV/VUV fluxes will be difficult. New reactor configurations, chemistries and power delivery schemes may be needed to obtain the needed independent control over radical, ion, and photon fluxes to the wafer (or other plasma facing materials).

One possibility for separately controlling ion and VUV fluxes in LTPs is using pulsed power. For short life-time states, which is usually the case for UV/VUV emission even with radiation trapping, photon fluxes to the wafer are closely aligned with power deposition. Since ions to the wafer have a finite transit time, there is some average of ion fluxes to the wafer over a pulsed period. These disparities enable some control of the ratio of photon-to-ion fluxes to the wafer, which may control synergistic reactions. (See Figure 5B-3.)

2. *How do photo-generated electrons and holes promote etching reactions, and can control of the plasma enable control of these etching reactions?*

VUV light can stimulate etching by several mechanisms. The most commonly studied and invoked process involves the formation of electron-hole pairs in non-metallic materials. Electrons and holes migrating to the surface can aid breaking of Si-Si bonds and/or cause desorption of products. In the example in Fig. 5B-4, the conduction band minimum and valence band maximum energy levels of a p-type semiconductor bend down at the surface in the absence of a plasma, due to Fermi level pinning at mid-gap by surface states. In the presence of a plasma, above-bandgap light (1.12 eV for silicon) creates electron hole pairs within the photon penetration depth. For photon energies just above the bandgap energy, the minority carrier (i.e., electrons for p-type semiconductors) will "fall" to the surface. With higher energy VUV photons, the excess energy released into "hot" electrons and holes allows the majority carriers to overcome the potential barriers and also reach the surface, while also slowing electron-hole recombination at defect sites, thereby increasing the effectiveness of charge carriers in enhancing surface chemistry. Higher energy carriers created by VUV light will also ionize, creating additional carriers. These effects might be further influenced by the thickness and composition of the etching surface layer containing electronegative species and perhaps negative ions. Furthermore, the degree of band bending depends on dopant concentration and light intensity. It is also likely that the ion bombardment that causes etching also modifies the surface and influences the photo-effects. Therefore, careful experiments to isolate the effects of dopant types and concentrations, photons, ions, electrons and adsorbates, carrier recombination rates, etc., combined with theory are needed to provide insights into this poorly understood aspect of plasma processing of semiconductors and enable the design of VUV emitting plasma sources to capitalize on (or deemphasize) these effects.

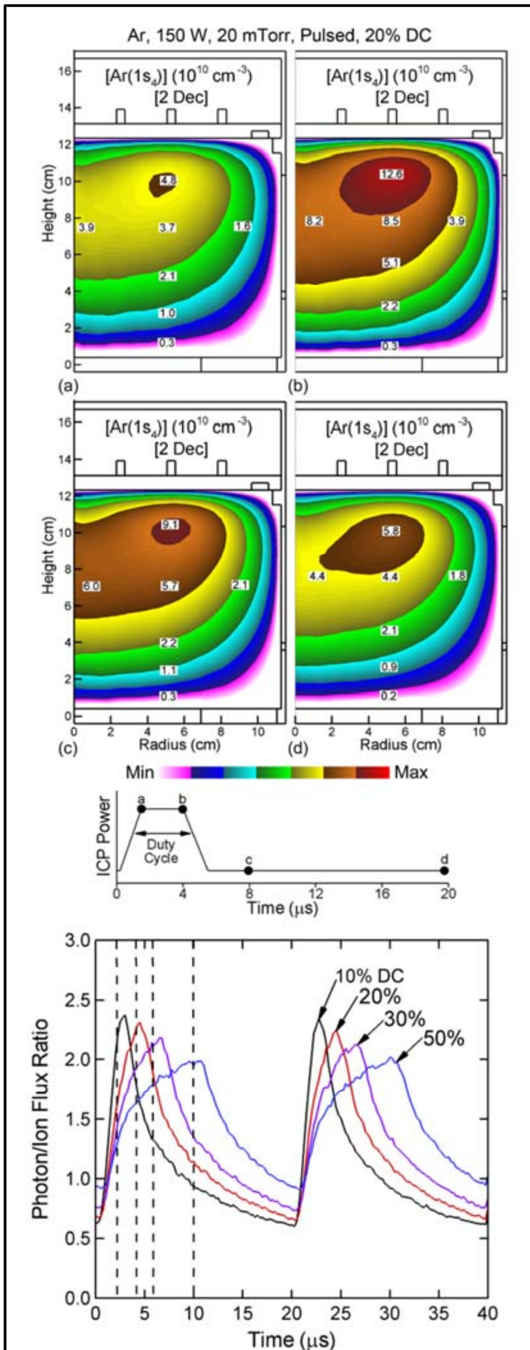


Figure 5B-3: Properties of a pulsed inductively coupled plasma (50 kHz) in 20 mTorr argon. (top) Density of Ar($1s_4$) resonant state at 20% duty cycle. (bottom) Ratio of VUV photon flux to ion flux onto the bottom substrate for different duty cycle. The vertical lines are the end of the power pulse. [121]

3. *What are other possible mechanisms for photo-assisted etching?*

VUV light can also stimulate etching by causing desorption of species at the surface. Direct substrate bond breakage can also aid in opening up the lattice, aiding in etchant (e.g., Cl or F) penetration and enhanced etching. Such a mechanism has been proposed, but there is little supporting evidence for this process. Existing carrier-mediated and photo-stimulated desorption mechanisms cannot produce yields in excess of unity. Yet it is reported that VUV light causes etching of semiconductors (Si in the presence of XeF_2 gas, Si in a chlorine plasma, and GaAs in the presence of Cl_2 gas) with yields of 100 per photon or more. Additionally, Cu in the presence of Cl_2 gas has also been found to etch with a yield of 2-10 per photon. [142] Hence, no existing mechanism can explain the large yields. These processes will feed back to the plasma by introducing fluxes of reactive species from the desorption process. These synergistic processes are, in principle, controllable by managing the UV/VUV fluxes produced by the plasma.

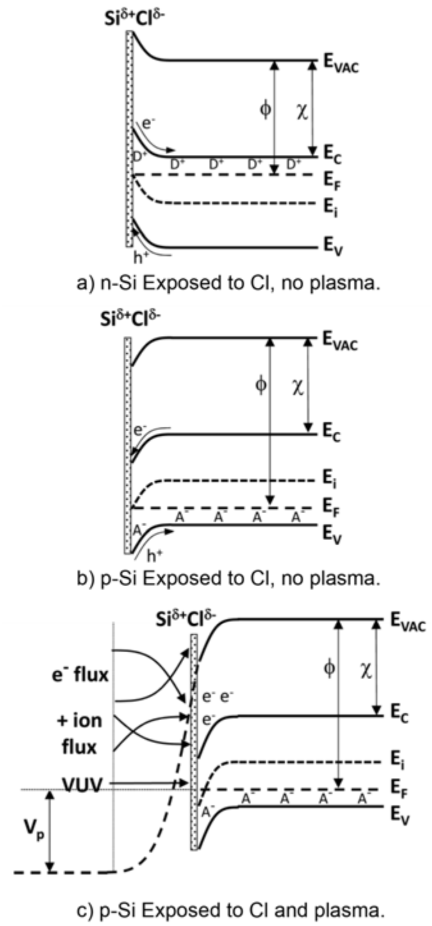


Figure 5B-4: Qualitative band diagram near the surface of chlorine-exposed *n*-type and *p*-type Si in the absence of a plasma and for *p*-type Si in the presence of a plasma. [126]

4. *How important is VUV induced creation of damage and defects?*

The energies of VUV photons exceed the bond strengths of semiconductors, as well as insulating materials. Hence, in addition to the ephemeral production of electrons and holes, VUV photons can also create long-lasting damage, including bond fissure and trapped charges, within the photon penetration depth. This can occur during etching as well as during plasma-enhanced chemical vapor deposition processes. The effects of UV and VUV light on insulating materials including photoresist, SiO_2, and porous SiOCH have been widely reported but are still relatively poorly understood. [129, 143, 144] For photoresist, the main effects involve roughening of the sides of the lithographically defined features during plasma etching. For the low dielectric constant SiOCH films, a similar erosion of the sidewall takes place, causing a loss of CH_3 groups and an undesirable increase in the dielectric constant.

5. *What are the effects of VUV light on processes at other plasma-facing surfaces and their feedback to the plasma?*

While photon-wafer interactions are the primary concern to device fabrication, it is also likely that photon interactions with the chamber walls affect plasma chemistry. As there is more area in contact with the plasma that is not wafer than is wafer, these interactions can have large consequences on plasma behavior. In addition to creation of secondary electrons by photo-electron emission, since the energy of positive ions bombarding the walls is usually relatively low, energetic photons may be the dominant cause of deposited etch products desorbing and reentering the plasma. These products have lower ionization potentials than most plasma feed gases, so even a small increase in their concentration could significantly alter the plasma density and electron energy distribution.

5B.c. Scientific Challenges and Research Opportunities

While it is possible that UV and VUV light could have some potential uses in plasma assisted etching and deposition, the negative effects likely outweigh the positive ones, at least at this stage. Consequently, the primary challenge is to eliminate, reduce, or control these effects. Within that charge is the need for a better understanding of the problems.

1. Quantifying plasma generated VUV fluxes to surfaces

It is often difficult to determine the absolute intensity of VUV light in a plasma. Observations through windows cut out the most important light at the higher energies. Consequently measurements must be made with the sensing device in contact with the plasma gas. The most relevant measurement is that made at the wafer surface; side views through differentially pumped chambers will not provide accurate measurements. Therefore, in-situ sensors capable of providing wavelength-resolved, absolute measurements of light intensities at wavelengths between ~50 and 300 nm are required. [118]

2. Improved understanding of the generation and propagation of VUV light in processing plasmas

A more thorough understanding of the generation and propagation of VUV light in LTPs is required. Both experiments and theory are needed. VUV absorption spectra of radicals and especially etching product fragments are mostly unknown but required to accurately assess the attenuation of light produced in the densest regions of the discharge as it traverses the plasma volume and reaches the substrate. With validated models, processes can be tailored to minimize VUV fluxes while maintaining required etching rates and other metrics. There are some potential benefits to pulsing the plasma power for reducing the ratio of VUV, while not sacrificing as much of a drop in deposition or etching rates. This is partly due to the fact that the high-energy electrons that produce VUV light lose energy rapidly after plasma power is switched off, while positive ions and low-energy electrons leave the plasma at a much slower rate. Such approaches have not been widely explored, either through experiments or simulations.

3. Validated mechanisms for VUV induced etching and defect formation are almost totally lacking

Mechanisms of VUV photon-plasma-adsorbate-surface interactions are critically lacking and will be required to mitigate unwanted photo-effects. Experiments both outside of the plasma and in the plasma are needed. Outside of the plasma, individual phenomena such as photodesorption of neutrals and ions need to be studied. Creation of defects such as trapped charges in insulators can also be clarified. Experiments with neutral beams of stable species and radicals, combined with wavelength variable photon beams, such as those supplied by a synchrotron, would provide for conditions approaching those in a plasma, but with more control. Such experiments would provide the kind of insights that were obtained with ion and neutral beam experiments carried out in early investigations of plasma etching.

Most importantly, more experimental investigations in plasmas are needed. The interplay between photons, ions, neutrals, and electric fields provides ample possibilities for combined effects. Indeed, there have been reports of synergism of ions and photons on the dielectric constant of SiOCH as well as the roughening of photoresist. [145] Anti-synergistic effects have also been found: ion bombardment or the presence of adsorbed oxygen have been found to slow the photoassisted etching of Si in a chlorine plasma. [11]

5B.d. Potential Impacts

It is likely that effects stimulated by the energy released by photons could cause detrimental damage during plasma enhanced chemical vapor deposition (PECVD), as well as a lack of etching fidelity, thereby limiting continued use of plasmas in semiconductor manufacturing. Conversely it is also possible that this alternative pathway for delivering energy to the surface could lead to beneficial desorption of an etching product and “disrupt” the ion-neutral synergy mechanism that has driven plasma etching since its inception. This could be of great importance as an ultralow-damage etching process for future device fabrication.

Though VUV photo-assisted etching of Si and other semiconductors may be of interest as an ultralow-damage etching process, the (111) sloped sidewalls are an undesirable effect that will likely interfere with many etching processes, especially atomic layer etching with low energy ions. Consequently, a deeper understanding of the synergistic effects of VUV light and radicals, ions, crystal surface, and sheath electric fields on plasma etching is critically important for future microelectronics processing. In particular, the photocatalytic VUV photon initiated etching process appears to be an important new phenomenon, worthy of study in its own right.

A thorough understanding of the generation of VUV light in processing plasmas, its transport to surfaces, and the complex chemistry and solid-state physics, including electronic effects, of the photon-surface interactions will be required to ensure that plasma processes, most importantly plasma etching, continue without limits in future semiconductor device manufacturing.

PRO 6: Develop novel institutional structures to meet emerging challenges of the field

6a. Summary

The CHIPS for America Act of 2022 is specifically intended "to develop onshore domestic manufacturing of semiconductors critical to U.S. competitiveness and national security." [146] A summary of this Act also notes a disconcerting trend in US manufacturing: "Only 12% of chips are currently manufactured domestically, compared to 37% in the 1990s, and many foreign competitors, including China, are investing heavily to dominate the industry. The United States also lacks capabilities to produce the most advanced chips at volume." [146] It should also be noted that "the cost of building and operating a fab in the U.S. is now 20 to 40% higher than in other countries." [147] The USA must regain its position as a top producer of the most advanced electronic devices and circuits, or it will place both national security and the economy at risk. The far reaching and visionary CHIPS for America Act of 2022 is aimed to help the USA remain secure and competitive internationally. It includes appropriations to (1) incentivize onshore manufacturing of semiconductor devices, circuits, and systems, (2) conduct research and development (R&D) into advanced semiconductor manufacturing, and (3) increase workforce development and training opportunities.

Advancements in plasma science and engineering are central to all three of these goals. Low temperature plasmas (LTPs) are an enabling technology for the manufacture of semiconductor devices. As articulated in the previous PROs, plasmas enable anisotropic etch and low temperature deposition of both well established and novel materials; they are used to clean and modify surfaces and to dope material surfaces; and they are used to make the UV, VUV, and EUV light for lithography. Plasmas allow fabrication at a near-atomic level and on a scale suitable for mass production, resulting in their use in about 40-45% of all device fabrication steps. However, the majority of individuals entering the semiconductor workforce do not have fundamental understanding of the science and applications of LTPs . [148]

To make significant advancements in low temperature plasma science and engineering (LTPSE) will require making substantial investments in the research infrastructure in the US. This includes basic and transitional research at universities and national laboratories as well as applied research at US corporations. Advancing LTPSE also requires an emphasis on workforce development. A vision for the needed advancement in basic and transitional LTPSE research is outlined in PROs 1 - 5. PRO 6 addresses two related challenges: the need for continuous improvement in institutional infrastructure to better address unprecedented challenges to conducting and commercializing groundbreaking research in LTPSE, as well as the need to recruit, educate, and deploy larger numbers of talented and motivated people from all backgrounds into the LTPSE field.

In some important ways, the present institutional structures have served the country well and continue to do so. Even so, the constituencies of the LTPSE field should be further enabled and encouraged to propose novel institutional structures aimed at even more effectively meeting the anticipated unprecedented challenges and opportunities. One group has stated a key question well:

> "All of the published proposals we have seen so far advocate spending more on research, training the workforce for the future, and leveraging the infrastructure that the writers either already have in place or hope to build. *But a question we should ask is what kind of next-generation research and development (R&D) infrastructure will be needed to meet future challenges* in the face of the technological and economic obstacles that lie ahead?" (Emphasis added) [149]

This question should be extended to also ask "what next-generation educational infrastructure will be needed" and which can be implemented today? The term *infrastructure* here refers both to physical facilities and institutional processes. Institutional processes would include, for example, collaborative programs between government, universities, and industry, master plans, and regular funded opportunities.

The challenges faced by those doing research and development in LTPSE today have scientific, intellectual, and financial elements. The challenges for those engaged in educating the next generation of the LTPSE workforce are also unprecedented. Few scientists and engineers have the wide-ranging expertise to carry out groundbreaking research leading to advances at the atomic scale while also being able to transition their discoveries to high volume manufacturing (HVM). This is because, in the context of the CHIPS Act, the LTPSE field is strongly multi-disciplinary with high level science challenges while implementation is capital intensive. These obstacles must be overcome in a fashion which more quickly translates scientific advances to commercialization The current compartmentalization of research performed in universities, national laboratories, and private industry does not accomplish this translational mission well enough today. Several major US corporations have noted this compartmentalization at conferences as part of encouraging enhanced collaboration and new, more effective, and sustainable business models. [149, 150, 151, 152, 147, 153] Infrastructure can greatly accelerate a community's ability to make progress by enhancing strengths while reducing known obstacles. *DoE and FES leadership is needed to both develop and implement these novel infrastructures for the well-being of the low temperature plasma science and engineering (LTPSE) community.* The direct result will be enhancement of semiconductor manufacturing capabilities in the US.

The next section provides background to the key questions for this PRO, including an overview of the unprecedented challenges of the field in research and development, and in educating a workforce ready to work on manufacturing the next generations of devices, circuits, and systems. LTPSE is foundational to semiconductor manufacturing. Adapting and creating new institutional infrastructures for LTPSE to meet these challenges should be a priority.

6b. Key scientific questions

1. *How can we respond to the unprecedented challenges in low temperature plasma science for microelectronics fabrication to develop new technologies in a strongly multidisciplinary field with both fundamental scientific and commercialization challenges?*
2. *How can we produce a workforce for U.S. industry that is knowledgeable about low temperature plasmas and their applications?*

6c. Challenges and Opportunities

Nearly half of all steps in fabrication of microelectronics devices utilize plasmas. Film deposition is performed by plasma based physical sputtering, plasma enhanced chemical vapor deposition (PECVD), or plasma-activated atomic layer deposition. Lithography is done by EUV photons generated by laser produced plasmas. Etching is done by reactive plasmas, including by plasma-activated atomic layer etching. LTPSE is the essential knowledge supporting every semiconductor fabrication facility, and underlying most advances in semiconductor manufacturing. LTPSE is the field responsible for designing and making the tools that enable device manufacturing. Some of the reasons it has become so challenging to advance LTPSE related to semiconductor manufacturing include:

1. The lengths scales involved span ~9 orders of magnitude – from the sub-nanometer features on a chip to the meter-scale size of the plasma chambers used.
2. The knowledge base required throughout the industry is strongly multi-disciplinary and interdisciplinary. Changes in one technology have ripple effects through other technologies. Expertise in virtually every discipline in science and engineering is required.
3. Research and development have become extraordinarily expensive. New semiconductor fabs cost more than ten billion dollars. To do relevant training and research at a similar technology level means having access to similar, very expensive, tools and personnel.
4. Finding optimal "recipes" (the workflow or steps for a plasma process) through trial and error or even ordinary design-of-experiments has become too slow and cost prohibitive as the number of possible recipes increases.
5. The pace of *Moore's Law* is unforgiving. The entire field is expected to double its capability every two years at the same or reduced cost and size. This requires a daunting influx of new ideas and understanding.

6. This *Moore's Law* progression has been in progress at commercial scales for the last 40 years. Those who have been working in the field throughout this progression are now retiring.
7. Device dimensions are reaching atomic scale making "simple" scaling by shrinking device dimensions no longer feasible. As a direct result, the industry is moving to new materials. [148, 149, 150, 151, 152] Many of those materials are incompatible with existing technologies.
8. There is insufficient diversity within the LTPSE field, which unfortunately also makes the field less attractive to significant sections of the potential workforce.
9. There are too few universities and community colleges able to teach relevant subject matter.
10. Many of the needed teaching materials for LTPSE as well as semiconductor manufacturing are either dated or have yet to be developed.
11. Semiconductor manufacturing has become "largely invisible (to most students and the public)" [153] and LTPSE has become even more invisible today.

Semiconductor manufacturing requires trained people. The nation faces a chronic shortage of engineers and scientists, and this is particularly acute in the field of LTPSE. Few universities in the US have even a single course on plasmas for semiconductor manufacturing, and few community colleges and trade schools offer courses focused on plasma materials processing. This situation has resulted in a lack of domestic students pursuing educational opportunities that lead to employment in the semiconductor industry at all levels, from technician to researcher, a situation that should be corrected.

US universities have attracted some of the most innovative individuals from throughout the world who have entered the semiconductor workforce. Many of the leaders of the US semiconductor industry came to the US as graduate students. With the lack of domestic students entering the field, the current semiconductor workforce is highly dependent on this international source of talent. Strategies are needed to increase the pipeline of domestic students at all levels entering the plasma focused semiconductor workforce while also attracting international talent.

The Semiconductor Industry Association (SIA) has produced a projection on the needed workforce for the semiconductor manufacturing industry due to the CHIPS Act. (See Figure 6-1.) Scientists and engineers who are conversant in LTPSE are critically important to both the R&D and operations roles which comprise more than half the projected 300,000 employees by the 6th year. By way of comparison, the US annually produces at most a few thousand scientists and engineers conversant in LTPSE today, many of them being non-domestic students educated at US universities. We are educating at least an order of magnitude too few people in LTPSE in the US compared to that needed by the semiconductor industry just for

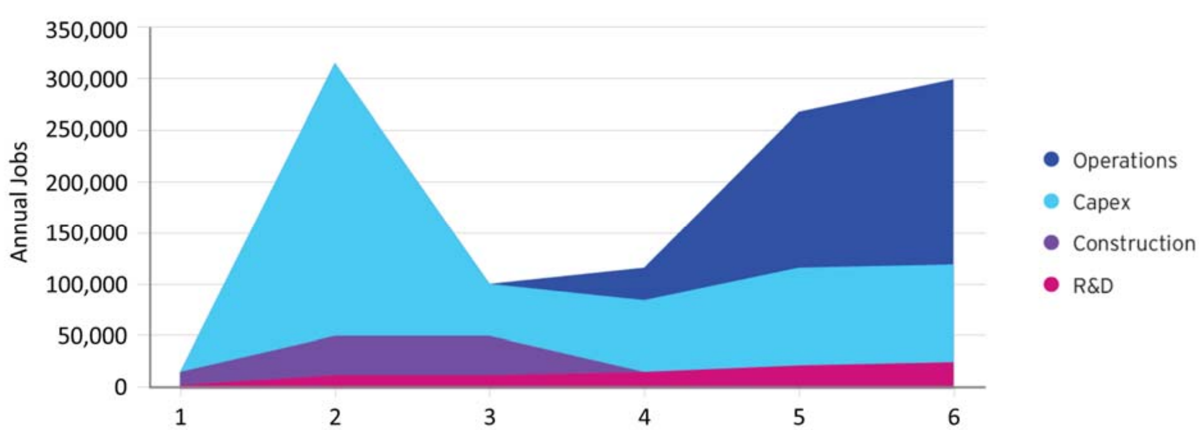


Figure 6-1: Projected total annual jobs impact of a $50 billion federal semiconductor manufacturing incentive program versus year after implementation. Plasma scientists and engineers are critically important to the R&D and operations roles which comprise more than half the projected employees. Graph reprinted with small alterations from the Semiconductor Industry Association [165].

this projected growth (not even considering replacing a retiring workforce). By not producing enough domestic educated engineers and scientists conversant in basic LTPSE, the nation faces several choices: (1) Hire people into those positions who are not sufficiently educated in LTPSE and train them on the job. This is largely the present model. This mode of operation wastes time and resources for US manufacturing, causing the country's output of innovation, technology, and chips to fall behind. (2) Greatly increase the pipeline of domestic students who wish to pursue careers in LTPSE and the semiconductor industry. (3) Return to more friendly immigration policies. This could widen the talent pool by encouraging top international students to study at US universities and transition to permanent positions at US semiconductor companies. (4) Hire foreign nationals educated at non-US universities into those positions. This could remain necessary even though it is not a top goal. In fact, the SIA has shown that the US semiconductor industry has had to increasingly rely on international students (mostly educated at US universities) to meet their workforce needs. (See Figure 6-2.) The US had roughly 4 times as many international graduate students as domestic students in STEM fields in 2016. [154]

There are currently proposals being put forward to address these challenges. (See for example [149], [151] regarding research infrastructure and [153] regarding education infrastructure. See also the CPP Strategic Plan [155] and [156].) Both the CHIPS Act and the related FABS Act [157] note that semiconductor manufacturing requires an extraordinarily well-trained workforce. With plasmas playing such an integral role in semiconductor manufacturing, it is crucial for a substantial fraction of its workforce to be conversant in how to best use plasmas in semiconductor manufacturing. This can only come about if we produce a workforce that is effectively trained in LTPSE.

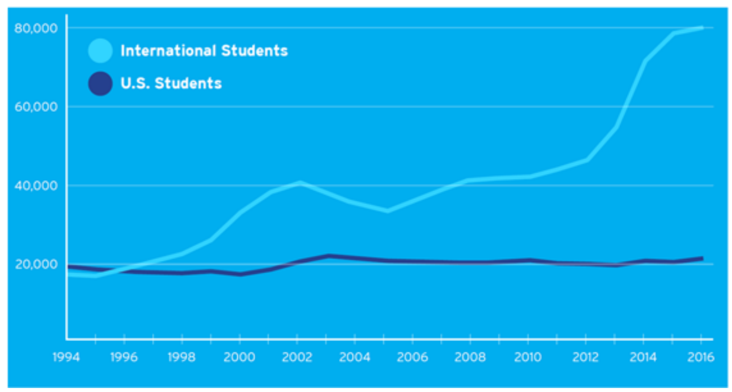


Figure 6-2: U.S. graduate education programs in the STEM fields of critical importance to semiconductor manufacturing are largely populated by international students. [154]

These workers are needed at all levels of education. High school graduates, technicians with a two-year Associates Degree, BS-level scientists and engineers, and those with a Masters or PhD degree are all critically needed. Educating these future leaders is challenging because available teaching materials in LTPSE at all levels are generally out of date. This is especially true of educational materials about plasmas for semiconductor manufacturing. This may be for several reasons, but one likely reason is because LTPSE is highly multidisciplinary. A second is that LTPSE research funding in the US has diminished significantly in the last decade, causing universities to focus on hiring their new faculty in other areas. There have also been far too few efforts to connect research institutions with semiconductor manufacturers and post-secondary institutions (and even K-12 institutions) to produce level-appropriate educational materials which benefit US industry.

Important Qualities of Proposed Solutions

The unprecedented challenges faced by the LTPSE community clearly indicate that enhanced and novel institutional infrastructures will be a crucially important part of the solution. This needed infrastructure can include an expansion of current programs, but such incremental changes are unlikely to produce the needed advances. Novel institutional infrastructures should be a top priority to address today's challenges.

The LTPSE community has identified several pressing needs in infrastructure and workforce development:

1. Improved capabilities to collaborate in research across university, national laboratory, and industry boundaries, both in emerging research areas and in existing fields. (See Fig. 6-3 for one example.)
    a. New institutional structures are expected to accelerate LTPSE research.
    b. Novel incentives for close partnerships between universities, national laboratories, and semiconductor manufacturing industry members are expected to speed transition of fundamental findings to industry.
2. Increased public and student awareness of LTPSE within semiconductor manufacturing. [153, 155, 156]
3. Increased pipeline of students ready to work in the semiconductor industry [148, 151, 153, 155, 156, 158]
    a. Educated to an industry acceptable level in LTPSE ("LTPSE conversant").
    b. Coming from appropriately diverse backgrounds. (Diversity in LTPSE in all dimensions.)
    c. Improved industry-university alignment in educational goals and outcomes.
4. Incentives to create new teaching materials, teaching collaborations / infrastructures / business models, and teaching technologies. Each should include an explicit ability to evolve rapidly and sustainably since the semiconductor manufacturing industry evolves rapidly.
5. A stable increase in funding for LTPSE research to encourage universities to hire in this field.

These needs and challenges indicate that novel infrastructures for the LTPSE community should:

1. Enhance access to resources for conducting relevant and groundbreaking research
    a. Make resources available on a competitive basis
    b. Enable access to specialized equipment, facilities, and expertise.
    c. Communicate research needs in LTPSE that are relevant to semiconductor manufacturing.
2. Encourage diversity and inclusion throughout the LTPSE community, including incentives to reach diversity goals.
3. Enhance collaboration among the LTPSE constituencies including, but not limited to, industrial researchers, academic researchers, and educators.
4. Support translational research at all levels.
    a. Enhance research dissemination between US-based companies, universities, and national laboratories.
    b. Encourage startups and/or new technologies to reach commercial maturity.
5. Create programs which encourage supporting and hiring greater numbers of faculty at universities, colleges, and trade schools who research and/or teach LTPSE related to semiconductor manufacturing. Encourage cross-over of industrial personnel into educational roles at all levels.
6. Engage with high school teachers to develop modules that introduce students to LTPSE.
7. Develop scalable programs to teach LTPSE at all levels and distribute those programs broadly.
8. Enlist and support efforts of plasma-based semiconductor manufacturing related professional societies and organizations.

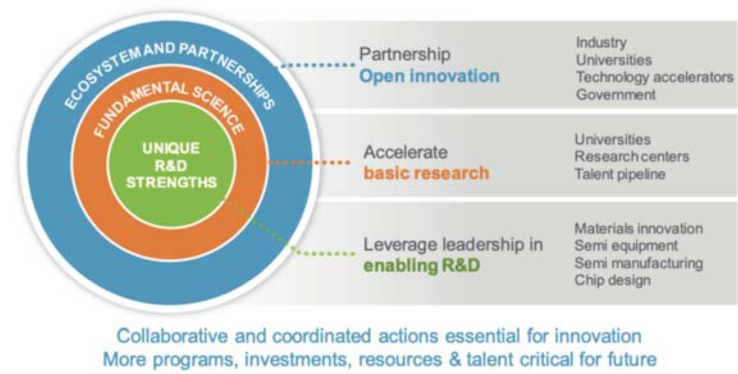


Figure 6-3: Companies across the semiconductor manufacturing spectrum are calling for enhanced collaboration and partnership opportunities. This graph, from Applied Materials, highlights thoughts on collaboration on multiple levels. taken from [[151], pg36].

There are numerous proposals to address these needs and challenges. We note a few here as examples. It has already been noted that there are too few academic groups in the US at higher educational institutions having involvement with semiconductor companies and their suppliers. One example of a proposed infrastructure modification to address this challenge has been put forward in a report by SEMI-ASA. [153] That report encourages cross-personnel appointments between industry, academia, and national labs to enhance collaboration, cross-fertilization, and education. Industry personnel might be granted release to teach at universities (i.e., teaching sabbaticals) and academic personnel be granted release to perform collaborative research in industry (i.e., industry sabbaticals). Another example could be focused Professional Masters programs. These degrees typically take 1 to 2 years beyond a Baccalaureate degree and typically include some type of project-based component similar to a thesis. In addition to being faster than a PhD program, Professional Masters programs tend to be more scalable to larger numbers of students.

Education at the BS level and below is also essential to support microelectronics manufacturing. Here the impediment is not usually the cost, but rather the ability of the school to create and teach the relevant curriculum. Partnerships with LTPSE capable educational institutions which would develop the curricular tools is one model which has enabled such programs to flourish. Another is the creation and maintenance of educational clearing houses devoted to a particular subject.

6d. Potential Impacts

Within the next five years the following goals should be achieved:

1. DOE should lead the effort to both find and implement novel infrastructures for conducting groundbreaking research in low temperature plasma science and engineering (LTPSE).
    a. The infrastructure should be participatory, scalable, sustainable, and at a national level for research and commercialization of LTPSE.
    b. The effort must engage the broad range of LTPSE constituencies including but not limited to academic institutions (from Carnegie R1 to primarily education oriented), established corporations, startups, and industry associations.
    c. The LTPSE community should be represented at the National Semiconductor Technology Center (NSTC) as well as any other novel infrastructure developed in the next 5 years. (See [146], [159] and [160].)
2. The number of programs at educational institutions that teach LTPSE directed at semiconductor manufacturing must increase substantially with a commensurate increase in students entering the field. This implies that the number of faculty devoted to such tasks will also need a significant increase.
    a. Provide incentives for domestic students to pursue graduate education in LTPSE. (See also the CPP Strategic Plan [155]and [156].)
    b. Continue to attract the best international students to US universities to study in LTPSE fields.
    c. Produce at least 100 PhD graduates / year in LTPSE by the 5th year.
    d. Enable stable and significant LTPSE research funding so that universities are motivated to hire in this area.
3. Every engineering and physical science department at US universities should aim to have at least a course or seminar in LTPSE related to semiconductor manufacturing.
4. Instructional materials in LTPSE related to semiconductor manufacturing appropriate for community colleges or even advanced high schools should be made widely available. Training resources on how to teach those materials must also be easily accessible.

Passage of the CHIPS for America Act of 2022 and related legislation is an unprecedented opportunity to make a major and lasting change to US-based semiconductor manufacturing. Since low temperature plasmas are critically important in semiconductor manufacturing, and plasma tools help determine the quality, quantity, and speed of chip production, renewed efforts should be directed into this field. These programs are an opportunity for institutional and infrastructural change which can help grow the US semiconductor manufacturing industry. Doing so will enable vibrant and cross-disciplinary research in LTPSE, new business models for sharing research costs and benefits, increasing speed to commercialization of new knowledge and technologies, and enabling a dramatic increase in our ability to educate in this area.

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Appendix A.

FES Workshop on Plasma Science for Microelectronics Nanofabrication

August 8-9, 2022
Hybrid Meeting: Gaithersburg Marriot Washingtonian Hotel & Zoom Virtual Meeting

Chair: David B. Graves, Princeton Plasma Physics Laboratory
Co-Chair: Mark J. Kushner, University of Michigan
Co-Chair: Catherine Labelle, Intel Corporation

Maintaining a robust domestic microelectronics supply chain will require major new investments in chip manufacturing capacity as well as advances in a multitude of fields in science and technology. One of the most important enabling technologies in microelectronics manufacturing is rooted in plasma science and the associated materials science and surface science that plasma activated processes enable. Plasma is an indispensable component of nanofabrication technology, being extensively used for thin film deposition, etching, and cleaning in conjunction with lithography for nanoscale patterning. The coming end of Moore's Law and the anticipated dramatic expansion in new materials in microelectronics manufacturing creates challenges and opportunities for plasma science and related nanofabrication technologies. New microelectronics applications will be based on materials with more complex, multicomponent structures. Understanding and controlling the interface between plasmas and these new material surfaces and structures will be needed to drive progress. Although plasmas are primarily thought of as underpinning the industry through materials fabrication, the extreme-ultra-violet (EUV) radiation enabling photolithography to define sub-10 nm features is generated by a laser-produced plasma. A workforce trained in these intrinsically multidisciplinary, plasma focused fields will be essential in maintaining US leadership in this indispensable technology.

The DOE 2018 Basic-Research-Needs (BRN) study on Microelectronics cited the challenges associated with continuing to improve computing power in the manner driven by Moore's Law. [1] As the report cites, achieving this goal will require new materials, synthesis technologies, architectures and algorithms, developed using co-design principles. To address the challenges and key questions discussed in the BRN, the plasma-based fabrication techniques that underpin the industry and the majority of materials synthesis processes must be integrated into the co-design process. This workshop will prioritize the science challenges that must be addressed to enable that integration.

Workshop Charge: The purpose of this workshop is to articulate the role of the DOE Office of Science, and Fusion Energy Sciences in particular, in advancing the plasma science required for new plasma-based semiconductor nanofabrication technologies. Among the objectives of the meeting are:

- Identify the fundamental plasma science areas (and their challenges) that are now supported or that could be supported by FES that will advance semiconductor nanofabrication capabilities in this strategic industry.
- Correlate the current research strengths supported by FES with semiconductor nanofabrication applications with the goal of prioritizing research activities in FES mission areas, including discovery plasma science, identifying where new capabilities are needed and where partnerships could be beneficial.
- Identify related areas of plasma science and plasma materials interactions that would benefit from a research program focused on the plasma science for semiconductor fabrication.
- Define plasma science's role in the co-design process required to vastly increase computing power.
- Propose a roadmap for supporting investigation of these science challenges and possible partnerships that will result in their translation to practice.

The goal is to provide FES with a set of prioritized research opportunities that can inform future research efforts in plasma-associated semiconductor nanofabrication science and build a community of next-generation researchers in this multidisciplinary area. The findings of this workshop meeting will be summarized in a report that should be submitted to FES within a month after the meeting.

Appendix B.

FES Workshop on Plasma Science for Microelectronics Nanofabrication Attendees

Workshop Chairs

Chair:	David B. Graves, Princeton Plasma Physics Laboratory (PPPL)
Co-Chair:	Mark J. Kushner, University of Michigan
Co-Chair:	Catherine Labelle, Intel Corporation

Plenary Speakers

Richard Gottscho, Lam Research
"Plasma Challenges for the Next Decade"

Gottlieb Oehrlein, University of Maryland
"Plasma Surface Interactions"

Uwe Kortshagen, University of Minnesota
Eray Aydil, New York University
"Plasmas for New Semiconductor Materials"

Eric Joseph, IBM
"The Future Evolution of Atomic Scale Processing to Enable New Materials and Devices"

Breakout Session Leads

Steven Shannon, North Carolina State University	Sources/Source Design
Laxminarayan L. Raja, University of Texas at Austin	Modeling
Eray Aydil, New York University	Diagnostics
Sadas Shankar, SLAC	CMOS & Beyond CMOS

In-person Attendees

Eray Aydil, New York University
Kallol Bera, Applied Materials
Peter Bruggeman, University of Minnesota
Richard Gottscho, Lam Research
David Graves, Princeton Plasma Physics Laboratory
Eric Joseph, IBM
Igor Kaganovich, Princeton Plasma Physics Laboratory
Uwe Kortshagen, University of Minnesota
Mark J. Kushner, University of Michigan
Catherine Labelle, Intel
Jose Lopez, Seton Hall University/National Science Foundation
Peter Mayer, ASML
Gottlieb Oehrlein, University of Maryland
Michael Purvis, ASML
Yevgeny Raitses, Princeton Plasma Physics Laboratory
Lax Raja, University of Texas Austin
Mohan Sankaran, University of Illinois
Joseph Sebastian, Hitachi
Sadas Shankar, SLAC
Steve Shannon, North Carolina State University
Russ Renzas, Oxford Instruments

Scott Walton, Naval Research Laboratory
Aaron Wilson, Micron
Tim Ziemba, Eagle Harbor

Virtual Attendees
Sumit Agrawal, Colorado School of Mines
John Arnold, IBM
Farhat Beg, University of California, San Diego
Brian Bentz, Sandia National Laboratory
Venkat Bommisetty, Princeton Plasma Physics Laboratory
Robert Bruce, IBM
John Cary, Tech-X
Jane Chang, University of California, Los Angeles
Yuanning Chen, Microsol Technologies
Enam Chowdhury, Ohio State University
Vince Donnelly, University of Houston
Ashim Dutta, IBM
Sebastian Engelmann, IBM
Matt Hopkins, Sandia National Laboratory
Tom Jenkins, Tech-X
Brian Jurczyk, Starfire Industries
Michael Keidar, George Washington University
Daniel Main, Tech-X
Shashank Misra, Sandia National Laboratory
Sang-ki Nam, Samsung
Larry Overzet, University of Texas at Dallas
Gregory Parsons, North Carolina State University
Shahid Rauf, Applied Materials
Thomas Schenkel, Lawrence Berkeley Laboratory
Shane Sickafoose, Sandia National Laboratory
John Verboncoeur, Michigan State
Mingmei Wang, Tokyo Electron America

Department of Energy Attendees
Nirmol Podder, Fusion Energy Sciences
John Mandrekas, Fusion Energy Sciences

Appendix C.

FES Workshop on Plasma Science for Microelectronics Nanofabrication Agenda

Monday, August 8th

7:30 – 8:00 am	Breakfast @ hotel	
8:00 – 8:20 am	Kickoff/Intro	Mark, David, Cathy
8:20 – 8:30 am	FES perspective	Jim Van Dam
8:30 – 9:00 am	Plenary: Plasma Challenges for the Next Decade	Richard Gottscho
9:00 – 9:30 am	Plenary: Plasma Surface Interactions	Gottlieb Oehrlein
9:30 – 10:00 am	Break	
10:00 – 10:30 am	Plenary: New Materials	Eray Aydil & Uwe Kortshagen
10:30 – 11:00 am	Plenary: CMOS & Beyond	Eric Joseph
11:00 – 11:30 am	Open discussion & Breakout org/assignments	Mark, David, Cathy
11:30 am–12:30 pm	Lunch @ hotel	
12:30 – 2:00 pm	Breakout session #1 • 2 sessions in parallel	
2:00 – 2:30 pm	Break	
2:30 – 4:00 pm	Breakout session #2 • 2 sessions in parallel	
4:00 – 4:30 pm	Break	
4:30 – 6:00 pm	Breakout session report-outs • 15 min per breakout • 30 min of final discussion w/everyone	Breakout leads
6:00 pm	Workshop Close	

Tuesday, August 9th

7:30 – 8:00am	Breakfast @ hotel
8:00 – 10:00am	Working session #1
10:00 – 10:30am	Break
10:30am – 12:00pm	Working session #2
12:00 – 1:00pm	Lunch
1:00 – 2:30pm	Working session #3
2:30 – 3:00pm	Break
3:00 – 4:30pm	Working session #4
4:30 – 5:00pm	Summary & workshop close

Appendix D.

List of Figures