Investigation of Co-Evaporated Bi_2Te_3 Thin Films on HD-4110 Polyimide for Thermoelectric Micro-Generators

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Introduction

Motivation:

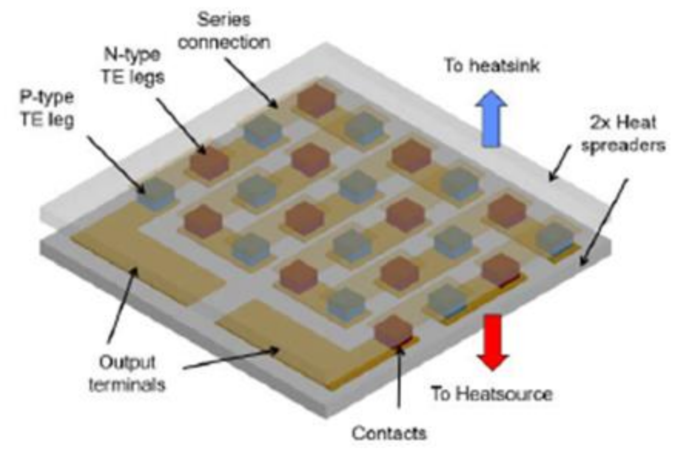
- Rising energy consumption has created a demand for sustainable, self-powered electronics.
- Thermoelectric micro-generators (μTEGs) function as self-powered sensors in applications for wearable technology and internet of things (IoT) devices.

Background:

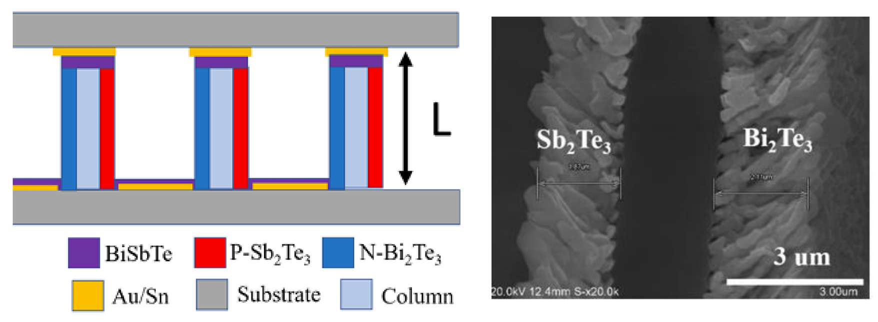
- Thermoelectric (TE) performance is measured by a TE figure of merit, ZT, shown below, where α_s is Seebeck coefficient, κ is thermal resistance, and ρ is electrical resistivity.
- Bi_2Te_3 is used due to its high ZT value compared to other materials, at room temperature.
- Thin film μTEGs are favored for their compact size, affordability, and flexibility vs bulk TEGs.
- Flexible thin film μTEGs use standard polyimide (PI) substrates which typically lack patterning.
- Elevating TE leg height to over 30μm is preferred to increase thermal resistance across μTEGs, shown in TEG power output equation below.
- Increasing the TE leg height will also allow for increased area available for TE thin film, increasing packing density of the μTEG device.

$$ZT = \frac{\alpha_s^2 \kappa}{\rho}$$

$$P_{TEG} = \overbrace{\left(\frac{\alpha_s^2}{2\rho}\right)}^{\text{Power factor}} \underbrace{\left(\Delta T_{total} \frac{R_{th_{couple}}}{R_{th_{total}}}\right)^2}_{\text{Temperature across thermocouple}} \overbrace{\left(\frac{A_{leg} N_{legs}}{L_{leg}}\right)}^{\text{Thermocouple geometry}}$$



Example of a standard lateral μTEG structure [1].



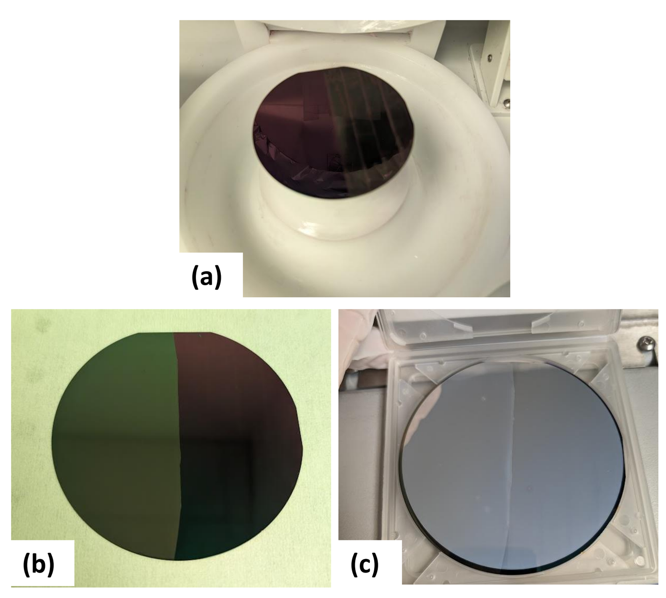
Vertical μTEG structure where the column defines the thermocouple length rather than film thickness, enabling high thermal resistance while maintaining thin film fabrication advantages, left [2]. Close up of deposited films on column showing non-planar crystal orientation, right [2].

Method Overview

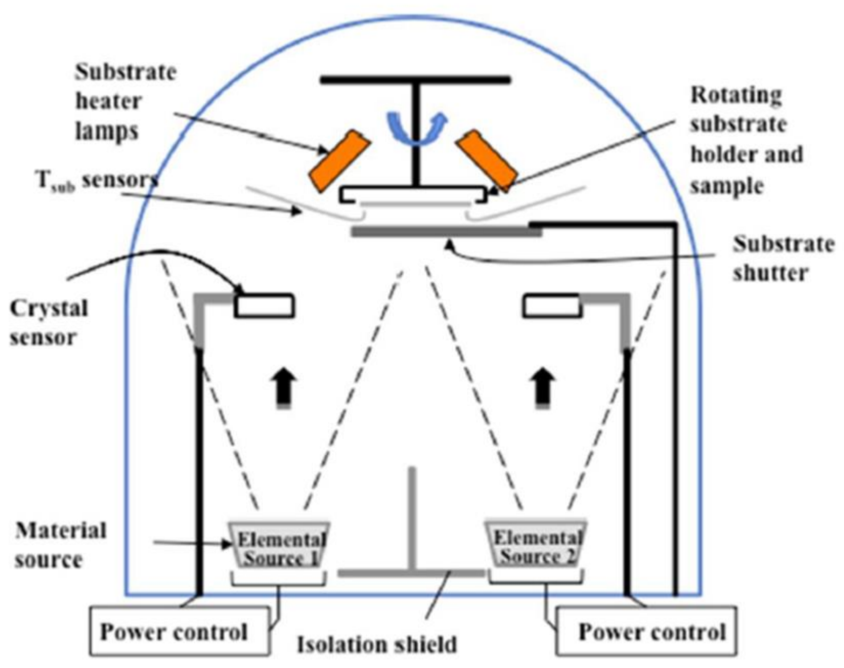
Processing Steps:

1. PI HD-4100 spun onto half of 4" Si wafers with a 500nm oxide layer
2. Wafers are soft baked at 85°C for 3 min, followed by 95°C for 3 min
3. PI films are cured at 200°C for 30 min, followed by 375°C for 1 hour
4. A Cr adhesion layer (50Å) and Bi_2Te_3 TE film (0.9μm) were deposited on all wafers by thermal co-deposition at a substrate temperature of 260°C

- Film properties of Bi_2Te_3 were measured on both PI and oxide layers.



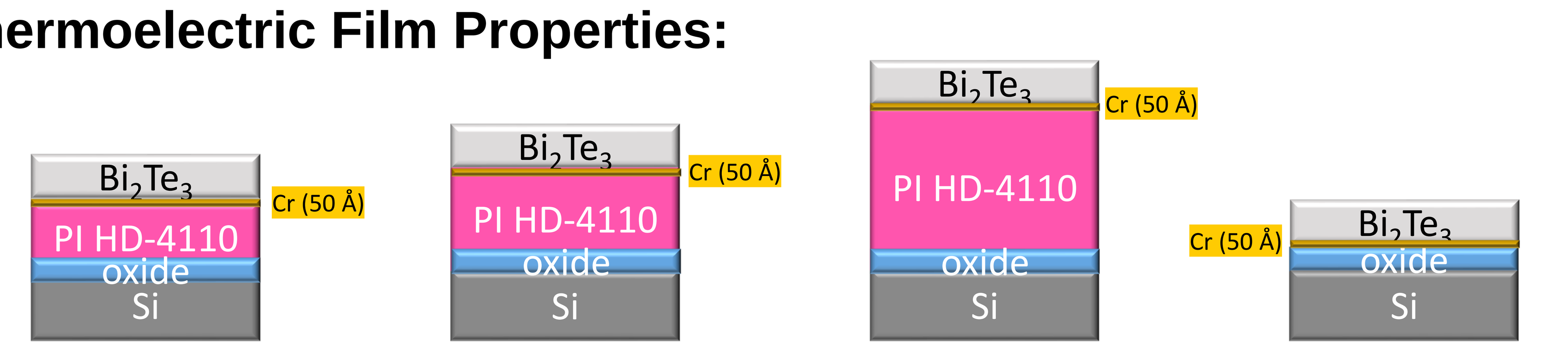
Wafer during steps 1 (a), 3 (b), and 4 (c).



Schematic of thermal co-evaporation system [3].

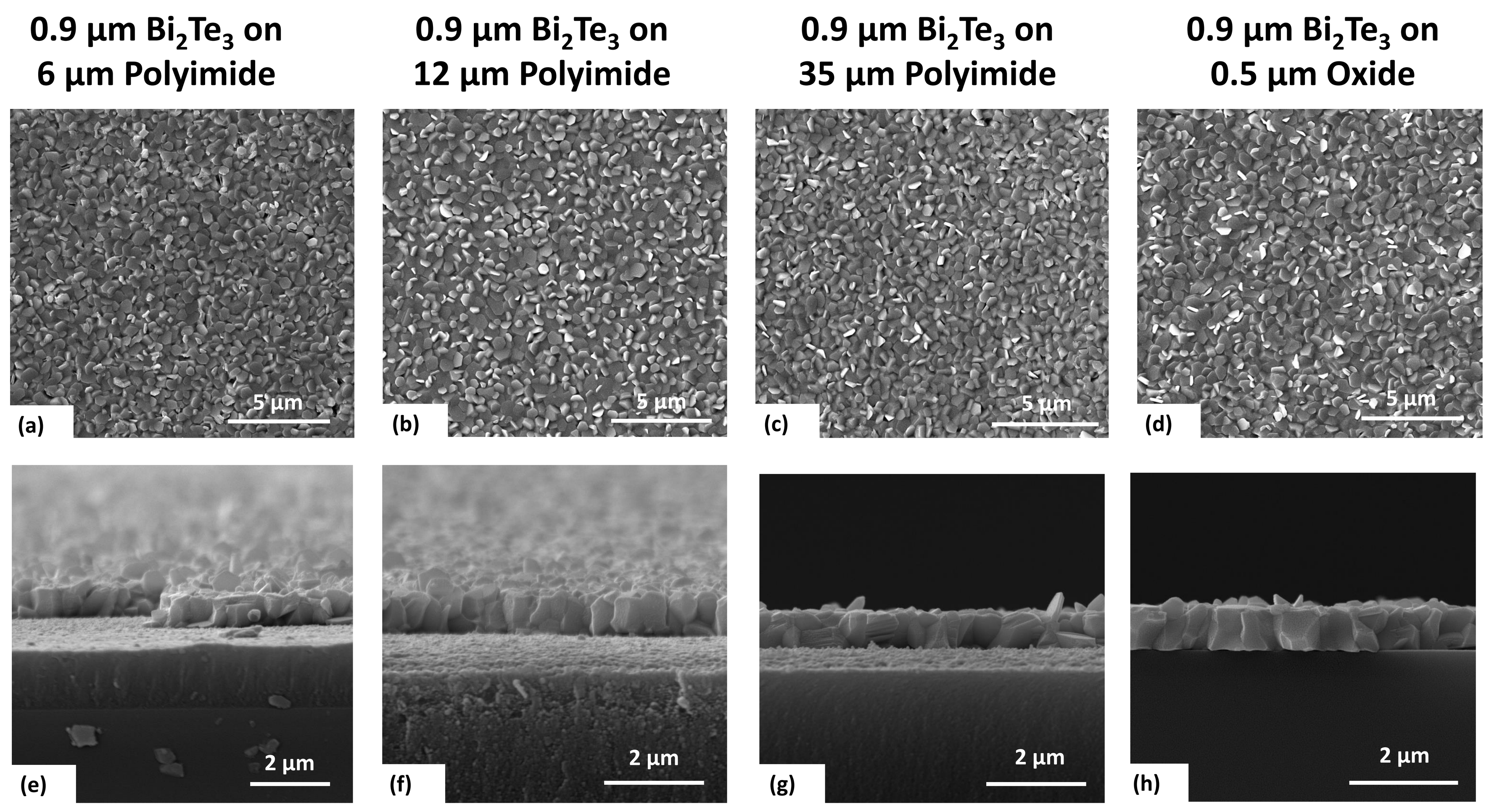
Results

Thermoelectric Film Properties:



$t(Bi_2Te_3)$ = 0.9 μm	$t(Bi_2Te_3)$ = 0.9 μm	$t(Bi_2Te_3)$ = 0.9 μm	$t(Bi_2Te_3)$ = 0.9 μm
t(PI) = 6 μm	t(PI) = 12 μm	t(PI) = 35 μm	t(oxide) = 0.5 μm
ρ = 9.9 μΩ-m	ρ = 10.7 μΩ-m	ρ = 11.8 μΩ-m	ρ = 24.5 μΩ-m
α_s = -168 μV/K	α_s = -167 μV/K	α_s = -184 μV/K	

Diagram showing thickness of each sample and its corresponding measured electrical resistance and Seebeck coefficient of Bi_2Te_3 films on varying thickness PI and oxide layers. Seebeck was not be measured on oxide because the adhesion was too poor.



Top view (a-d) and cross section (e-h) views of Bi_2Te_3 thin film on polyimide and oxide layers.

SEM Grain Size Analysis & EDS Elemental Composition

Grain analysis was measured by average grain size – Intercept ASTM method.

Layer under TE film	Layer thickness (μm)	Average grain size (nm)
PI	6	29 ± 3.0
PI	12	33 ± 3.0
PI	35	36 ± 0.1
Oxide	0.5	25 ± 1.4

Table showing average grain size measurements of Bi2Te3 films.

Flux Ratio (Bi:Te)	Atomic composition (%, Bi:Te)
1:3	40:60

Table showing flux ratio and atomic composition of Bi_2Te_3 TE film.

Electrical Resistivity & Seebeck Coefficient

$$R_s = \rho t \qquad \Delta V = \alpha_s \Delta T$$

Sheet resistance of Bi_2Te_3 deposited films was measured using a four-point probe and resistivity was calculated using the relationship above, left, where R_s is sheet resistance, ρ is electrical resistivity, and t is thickness of the thin film. Seebeck coefficient was determined using voltage probes and thermocouples to measure the voltage and temperature difference across the sample, equation shown above, right.

Discussion & Conclusions

- TE film Bi_2Te_3 was deposited over PI HD-4110 of varying thickness and oxide layers.
- Atomic composition of the Bi2Te3 film was 40:60, Bi:Te, which is the ideal ratio.
- The adhesion of TE films was much better on PI than oxide.
- TE film morphology (grain structure and orientation) and electrical resistivity did not change substantially with varying PI thickness (thicker PI produced grain sizes that were on average only ~10% larger).
- TE films deposited on oxide had on average a grain size about 15% smaller than those on PI and were found to have slightly higher electrical resistivity.
- Seebeck coefficient was similar on all PI thicknesses and measured to be -172±10μV/K on average.

Future Work

- Make patternable PI HD-4110 ramps for μTEG device fabrication.
- Altering the height of these PI ramps will allow for thin film TE material to be deposited over tall PI structures and optimal slope height will be determined for best performance.
- Increasing the height will also allow for increased area available for TE legs, increasing packing density of the μTEG device.
- Patterning PI will be done using grayscale mask lithography to control the ramp slope for enhanced TE performance.

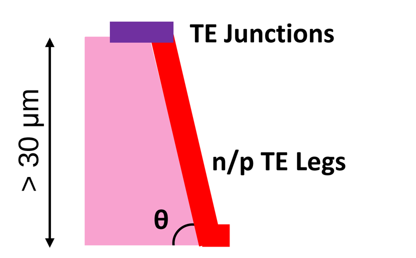


Diagram showing the PI ramp structure.

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