

Supplementary

Title: Realizing High Thermoelectric Performance at Ambient Temperature by Ternary Alloying in Polycrystalline $\text{Si}_{1-x-y}\text{Ge}_x\text{Sn}_y$ Thin Films with Boron Ion Implantation

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1. Thermal conductivity measurement

The ultrafast laserbased time-domain thermoreflectance (TDTR) technology, front heating front detection (FF) mode schematic diagram.

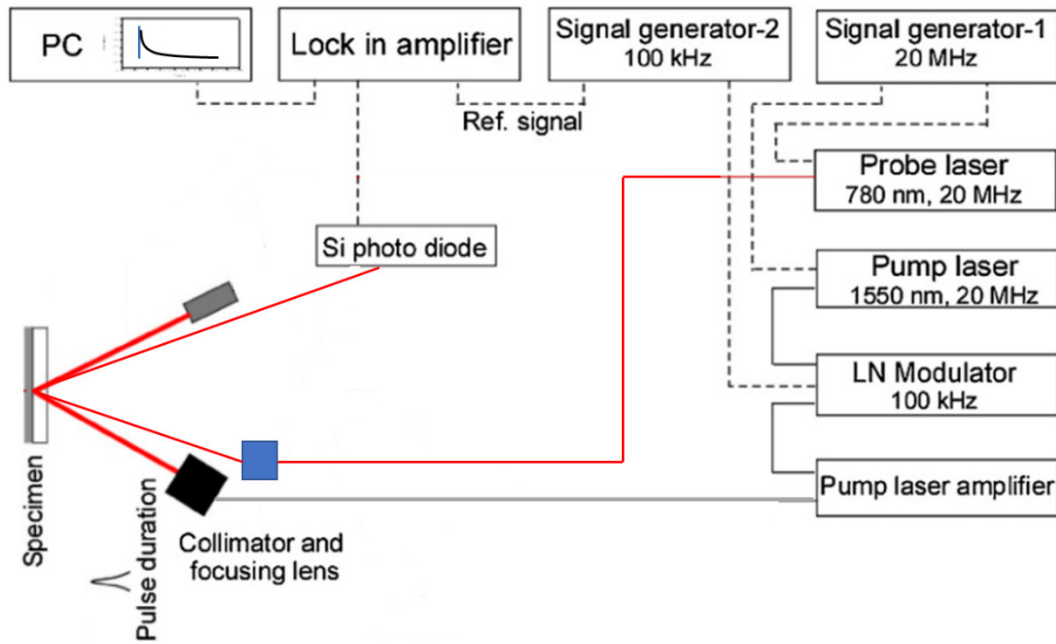


Figure 1. Schematic diagram of the FF laser pulsed thermoreflectance system.

Analysis test curve shown in Figure 2, use the formula¹

$$T_f(t) = \frac{1}{b_f \sqrt{\pi t}} \left[1 + 2 \sum_{n=1}^{\infty} \gamma^n \exp\left(-n^2 \frac{\tau_f}{t}\right) \right]$$

Get the sample thermal permeability $b = 1332 \text{ Js}^{-0.5} \text{ m}^{-2} \text{ K}^{-1}$

Use $\kappa = b^2 / \rho c$, here for $\text{Si}_{0.864}\text{Ge}_{0.108}\text{Sn}_{0.028}$, $\rho = 2786 \text{ kg/m}^3$, $c = 587.8 \text{ J/kgK}$

Get thermal conductivity $\kappa = 1.1 \text{ W/mK}$

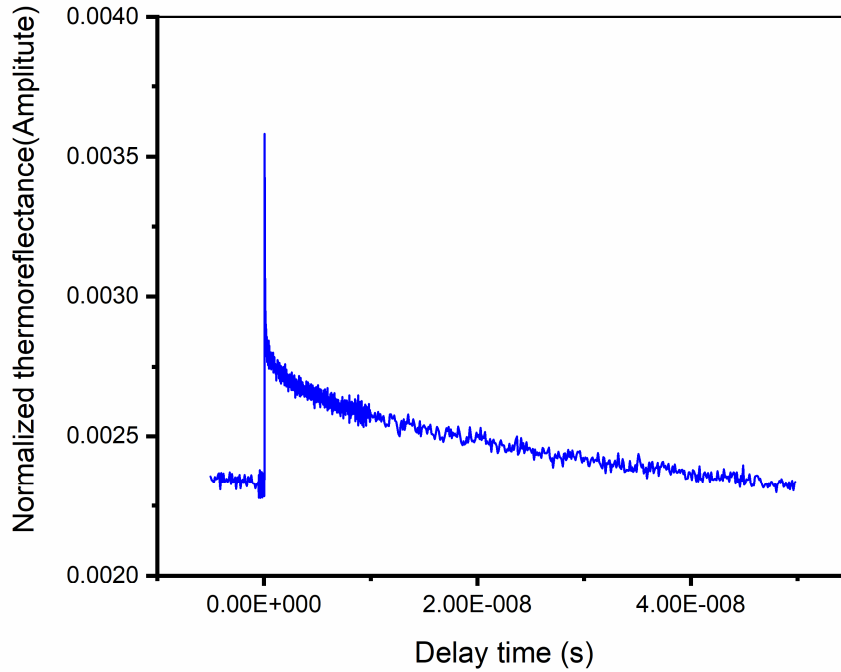
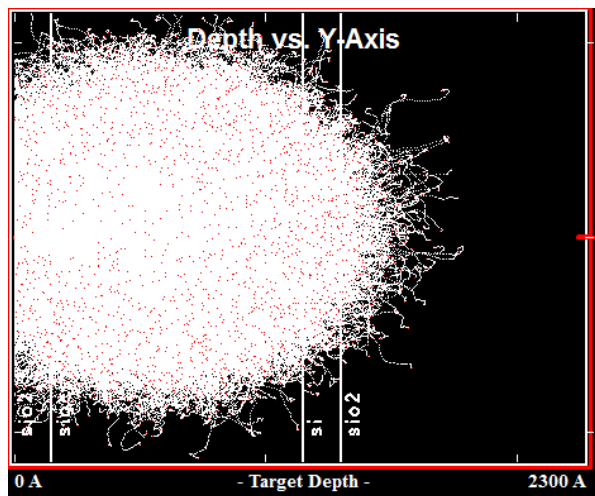


Figure 2. Temperature history curve of the 100 nm Mo film on 1100 deg C RTA $\text{Si}_{0.864}\text{Ge}_{0.108}\text{Sn}_{0.028}$ film.

2. SRIM ion implantation simulation

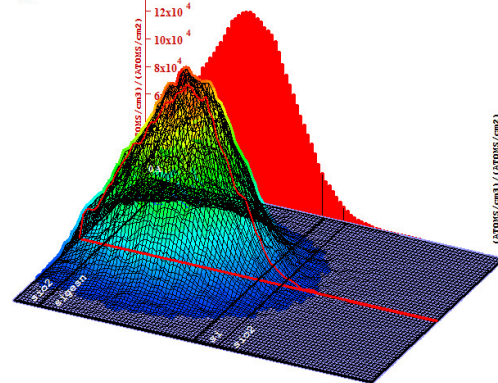
The SRIM simulation was performed for layers of the structure shown in Figure 3. First the projected range versus implantation energy was computed for the Boron ions in the amorphous $\text{Si}_{0.864}\text{Ge}_{0.108}\text{Sn}_{0.028}$ material to determine the nominal implantation energies (16 KeV) to be used. Before implantation, the simulated carrier concentration of the amorphous $\text{Si}_{0.864}\text{Ge}_{0.108}\text{Sn}_{0.028}$ is about $9 \times 10^4 \text{ atoms cm}^{-2}$, then with appropriate dose numbers $2 \times 10^{15} \text{ atoms cm}^{-2}$, the simulative maximal concentration is approximately $1.8 \times 10^{20} \text{ atoms cm}^{-2}$. After implantation, 15-second 900, 1000, 1100 and 1150 °C rapid annealing process was chosen to regulate the distribution of carrier concentration from 10^{19} to $10^{20} / \text{cm}^3$.



Ion Distribution

Ion Range = 655 A
Straggle = 276 A

Skewness = 0.037
Kurtosis = 2.519



Plot Window goes from 0 A to 2300 A; cell width = 23 A
Press PAUSE TRIM to speed plots. Rotate plot with Mouse.

Ion = B (16. keV)

Figure 3. Simulated B-ion implantation depth and distribution profile in $\text{Si}_{1-x-y}\text{Ge}_x\text{Sn}_y$ layer.

Table1. The sputtering parameters for depositing Si, Si_{0.864}Ge_{0.108}Sn_{0.028}, and SiO₂ films

Deposited layer	RF power (W)	Deposition rate (nm/min)	Deposition time(s)	Thickness (nm)
Si buffer	Si 150	2.80	313	15
Si _{0.864} Ge _{0.108} Sn _{0.028}	Si 150	2.80	1790	96
	Ge 10	0.35		
	Sn 3	0.09		
SiO ₂	SiO ₂ 150	2.92	309	15

Reference

1. Baba, T. Analysis of One-dimensional Heat Diffusion after Light Pulse Heating by the Response Function Method. *Japanese Journal of Applied Physics* **48**, 05EB04 (2009).