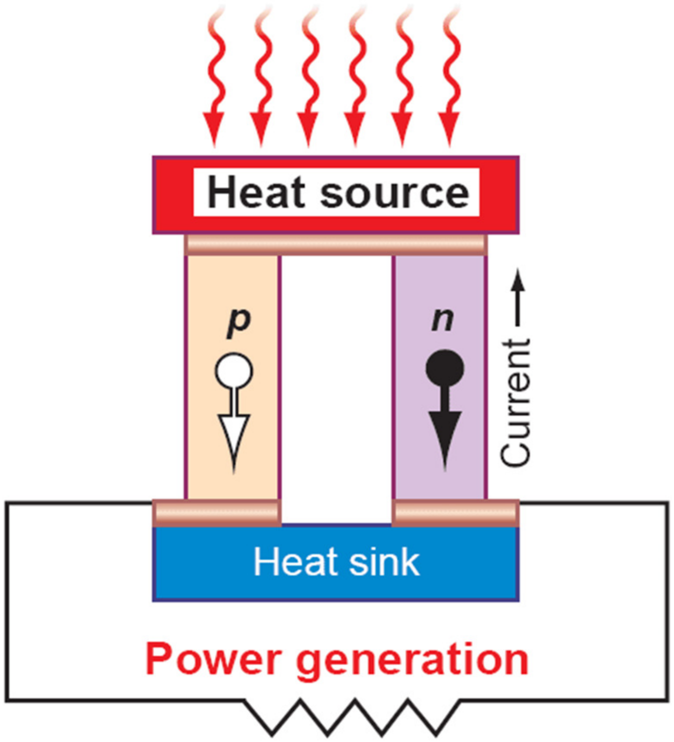
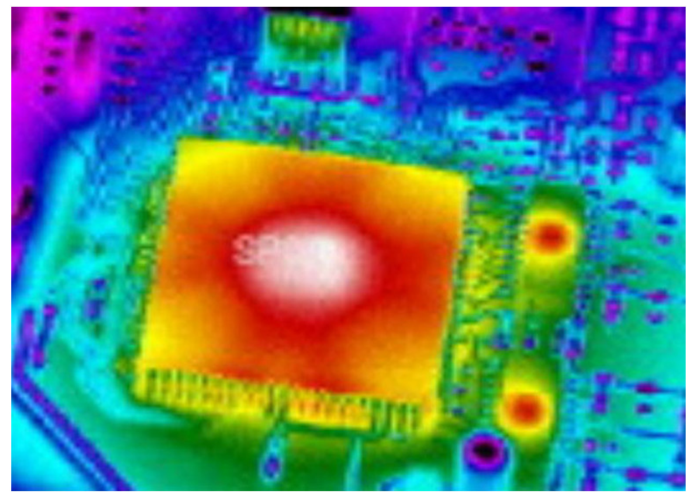
Thermal Conductivity of Amorphous Si and Ge Thin Films

Yibin Xu
National Institute for Materials Science, Japan

Thermal management issue for thin film



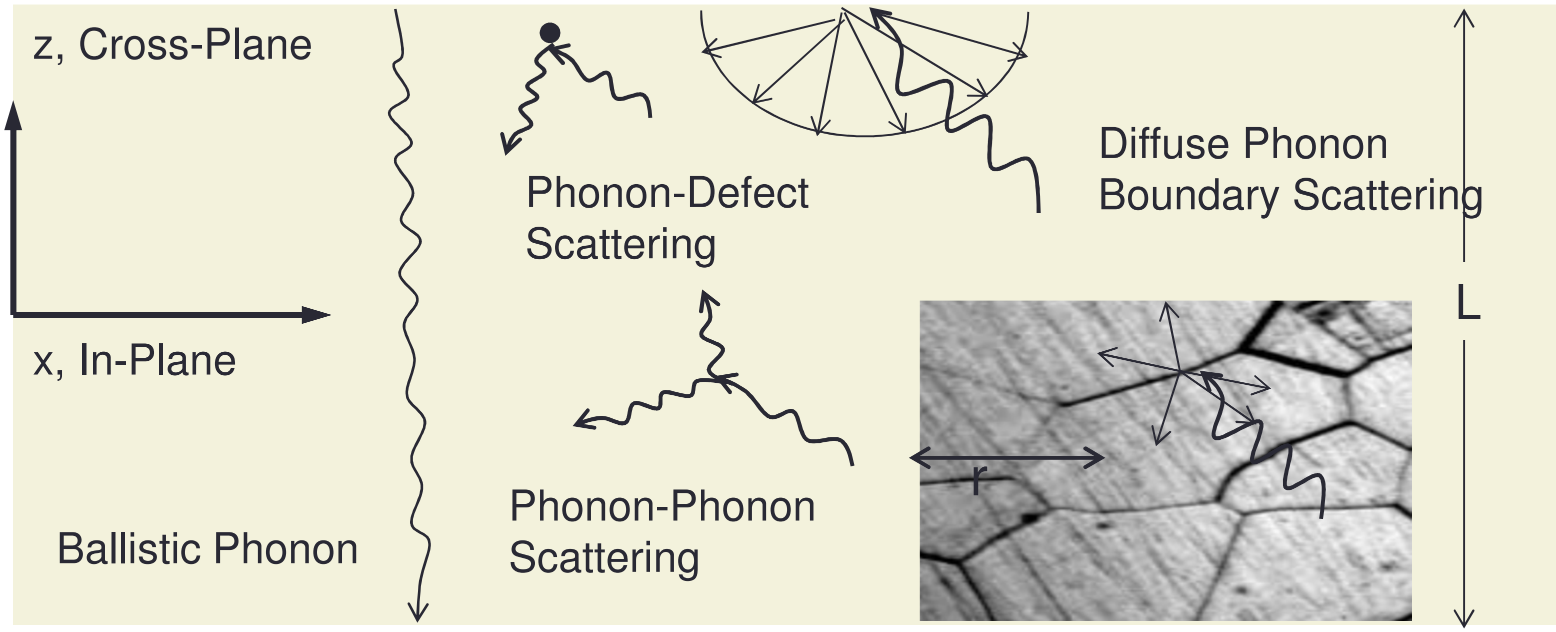
Thermoelectric devices



Thermal management

The transport forms of phonons has a great impact on the design of nanostructured thermoelectric materials with reduced thermal conductivity, as well as heat dissipation in electronic and photonic devices.

Phonon transportation in thin film



thermal conductivity :

$$k(T) \propto \int_{\lambda} C_{v,\lambda}(T) v_{\lambda}^{2} \tau_{\lambda}(T) d\lambda$$

$$k(T) = f(L, r, \rho_{imp}, v, T)$$

$Matthiessen's\ rule : \tau^{-1} = \tau_{imp}^{-1} + \tau_{U}^{-1} + \tau_{B}^{-1}$

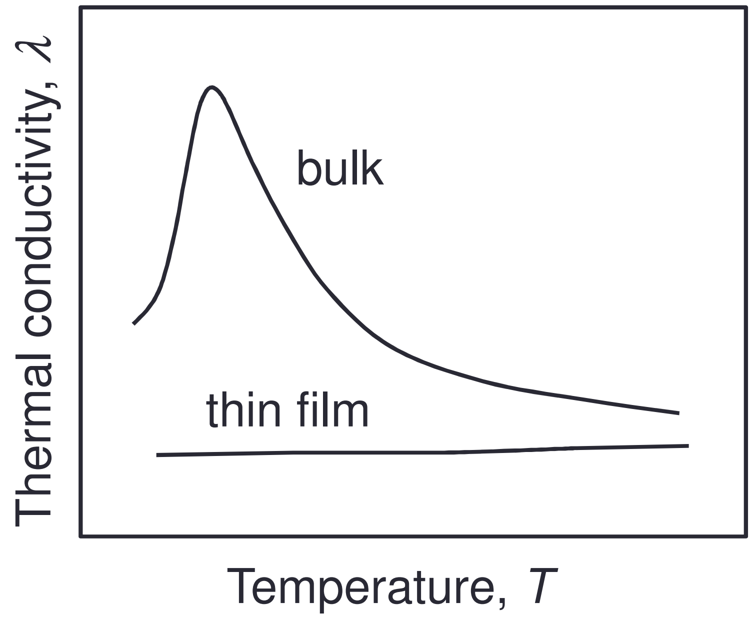
τ : phonon relaxation time;

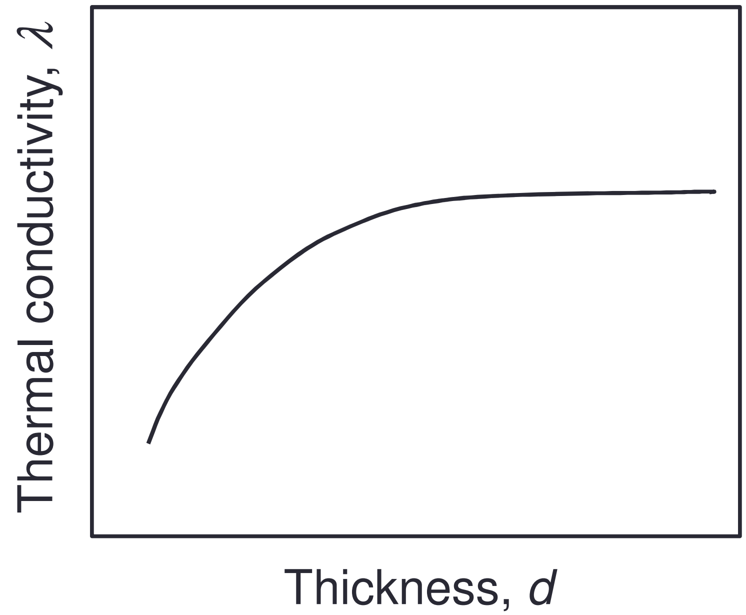
imp : impurity scattering;

U : Umklapp processes;

B : boundary scattering

Features of thermal conductivity of thin film





Film thickness dependence can be observed when $d \leq 10 \times l_{ph}$

How is amorphous thin film?

- easily synthesized
- extreme low thermal conductivity
- little knowledge of phonon distribution, transportation, etc.

Classic models describing heat conduction in amorphous solids

[1] Einstein model[1]: heat conduction in amorphous solids is described by a random walk of thermal energy between neighboring atoms vibrating with random phases.

[2] Minimum thermal conductivity model[2]: the minimum thermal conductivity is reached when the distance between collisions of elastic waves equals the wavelength of Debye waves.

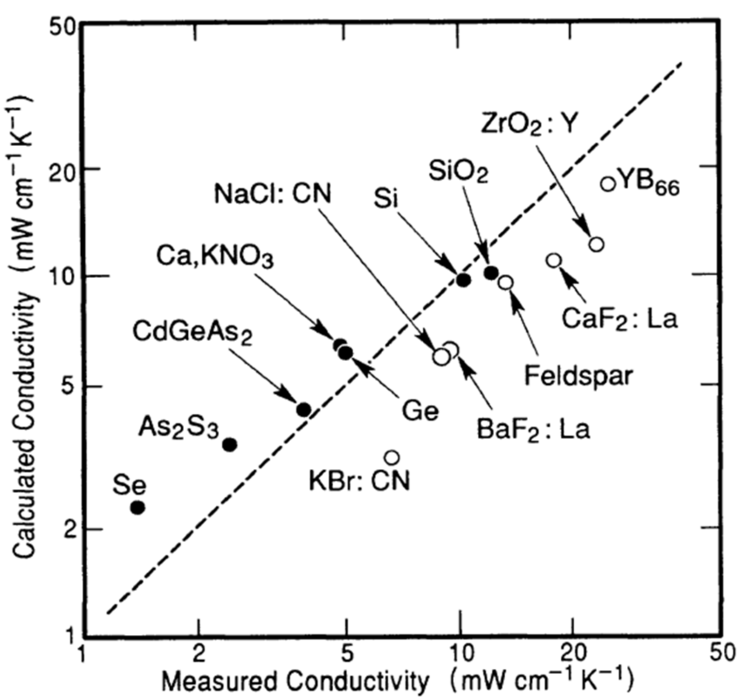


Fig. 1 Calculated minimum conductivity at 300 K versus the measured values for amorphous solids[3].

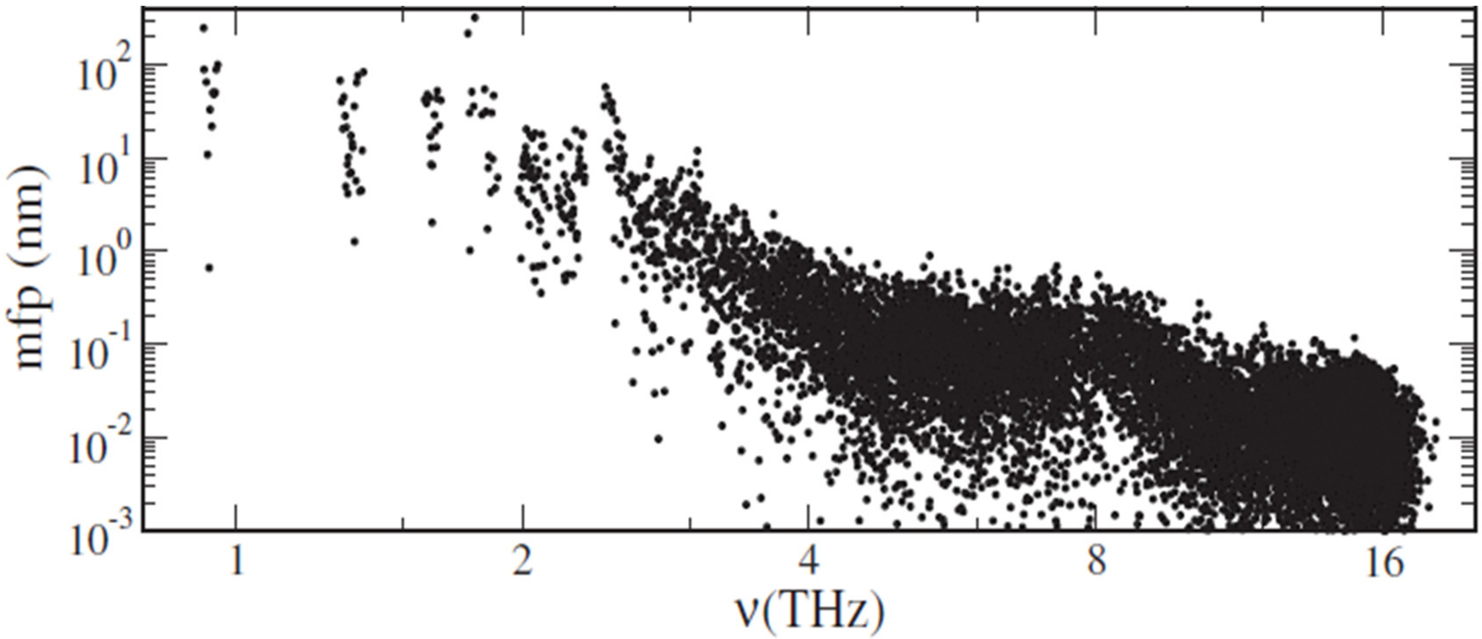
[1] A. Einstein, Ann. Phys. (Leipzig) **35**, 679 (1911).

[2] G. A. Slack, in Solid State Physics: Advances in Research and Applications, edited by H. Ehrenreich et al. (Academic, New York, 1979), Vol. 34, p. 1.

[3] D. G. Cahill, S. K. Watson, and R.O. Pohl, Phys. Rev. B **46**, 6131 (1992).

Phonon mean free paths in amorphous solids are several nm.

Existence of phonons with long mean free path predicted by MD simulation



Effective mean free paths of the vibrational modes of an a-Si in equilibrium MD simulations.

Y. P. He, D. Donadio, and G. Galli, Appl. Phys. Lett. **98**, 144101 (2011).

Purpose of research

Investigate the dependence of thermal conductivity of amorphous Si and Ge films on thickness and deposition conditions, and explore the nature of phonon propagating in amorphous solids.

Synthesis of Si(Ge) thin films

Au sensing film (150 nm)

Si(Ge) thin film (15,100,250 nm)

Ge(Si) substrate
(single crystal, 0.5 mm)

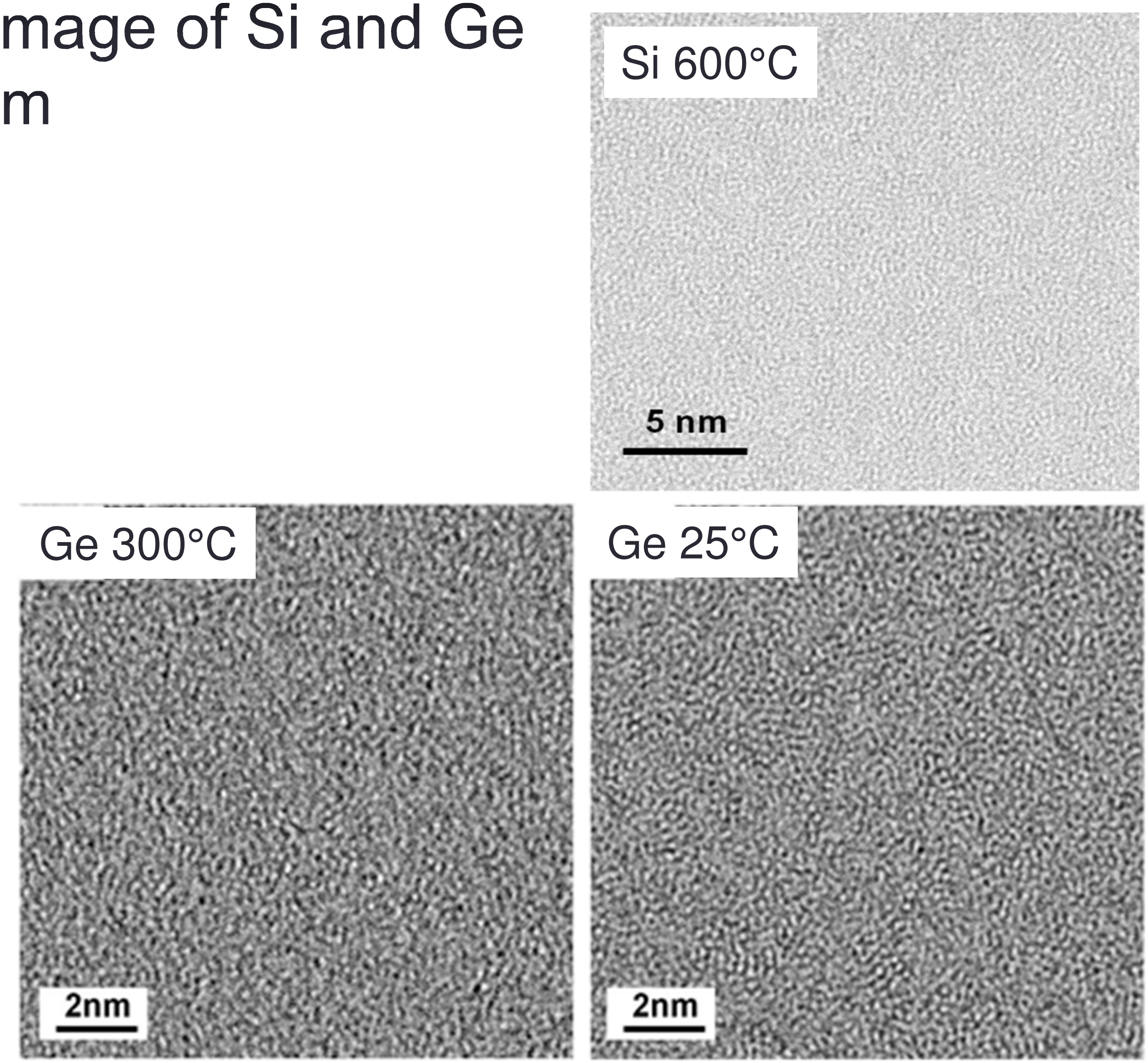
Magnetron sputtering

Deposition temperature

25 ℃ | 300 ℃ | 500 ℃ | 600 ℃

Deposition conditions

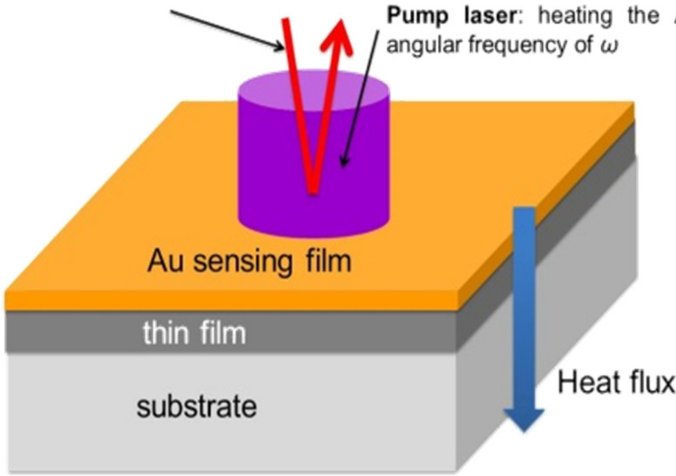
TEM image of Si and Ge thin film



Cross-plane thermal conductivity measurement (FDTR method)

Probe laser: the temperature at the surface of the Au film was measured using the thermoreflectance technique

Pump laser: heating the Au film with an angular frequency of ω



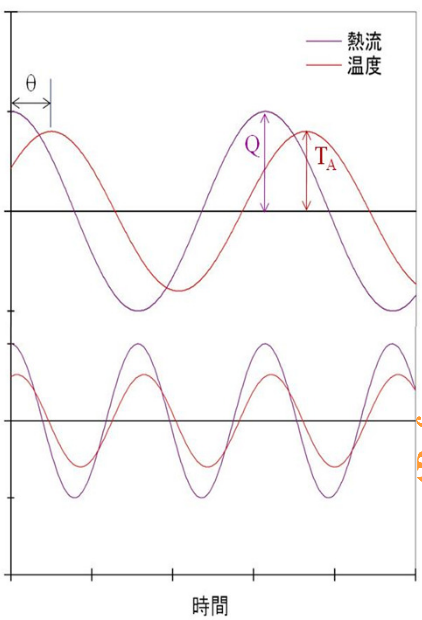
$$T(0)=\frac{q}{i\omega C_0}\left\{1+\left[\frac{\left[(1+i)\lambda_1k_1R-\left(1-\frac{\lambda_1k_1}{\lambda_2k_2}\right)\right]\sinh\left[(1+i)k_1d_0\right]}{\left[(1+i)\lambda_1k_1R-\left(1-\frac{\lambda_1k_1}{\lambda_2k_2}\right)\right]-\left(1+\frac{\lambda_1k_1}{\lambda_2k_2}\right)e^{2(1+i)k_1d_1}-(1+i)R\lambda_1k_1e^{2(1+i)k_1d_1}}+\frac{\left[\left(1+\frac{\lambda_1k_1}{\lambda_2k_2}\right)+(1+i)\lambda_1k_1R\right]\sinh\left[(1+i)k_1d_0\right]}{\left[(1+i)\lambda_1k_1R-\left(1-\frac{\lambda_1k_1}{\lambda_2k_2}\right)\right]e^{-2(1+i)k_1d_1}-\left(1+\frac{\lambda_1k_1}{\lambda_2k_2}\right)-(1+i)\lambda_1k_1R}-\cosh\left[(1+i)k_1d_0\right]\right]^{-1}\right\}$$

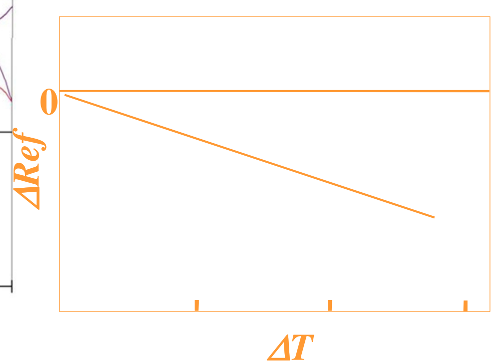
$$\text{where}\ ,k_j=\sqrt{\frac{\omega C_j}{2\lambda_j}}$$

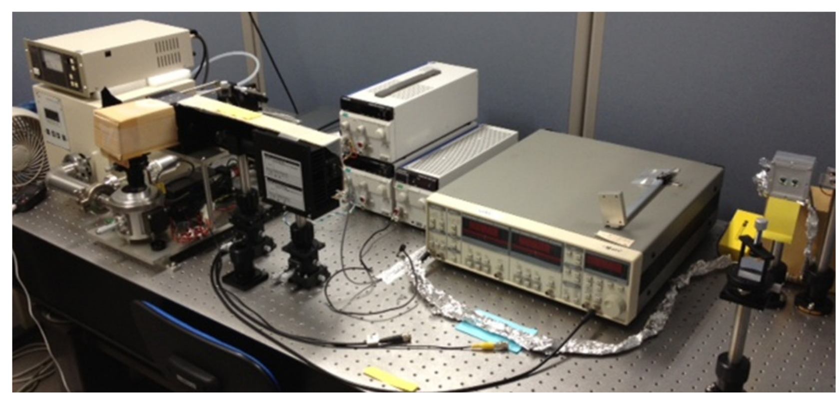
$$\text{when}\ \ k_1(d_0+d_1)<<1$$

$$\frac{T(0)}{qd_0}=\frac{e^{-i\frac{\pi}{4}}}{\sqrt{2\omega\lambda_2C_2}}+R+\left(1-\frac{\lambda_1C_1}{\lambda_2C_2}\right)\frac{d_1}{\lambda_1}+\left(\frac{1}{2}-\frac{\lambda_1C_1}{\lambda_2C_2}\right)\frac{d_0}{\lambda_1}$$

$$\frac{T_A\cos\theta}{qd_0}=\frac{\cos\left(-\frac{\pi}{4}\right)}{\sqrt{2\omega\lambda_2C_2}}+R+\left(1-\frac{\lambda_1C_1}{\lambda_2C_2}\right)\frac{d_1}{\lambda_1}+\left(\frac{1}{2}-\frac{\lambda_1C_1}{\lambda_2C_2}\right)\frac{d_0}{\lambda_1}$$



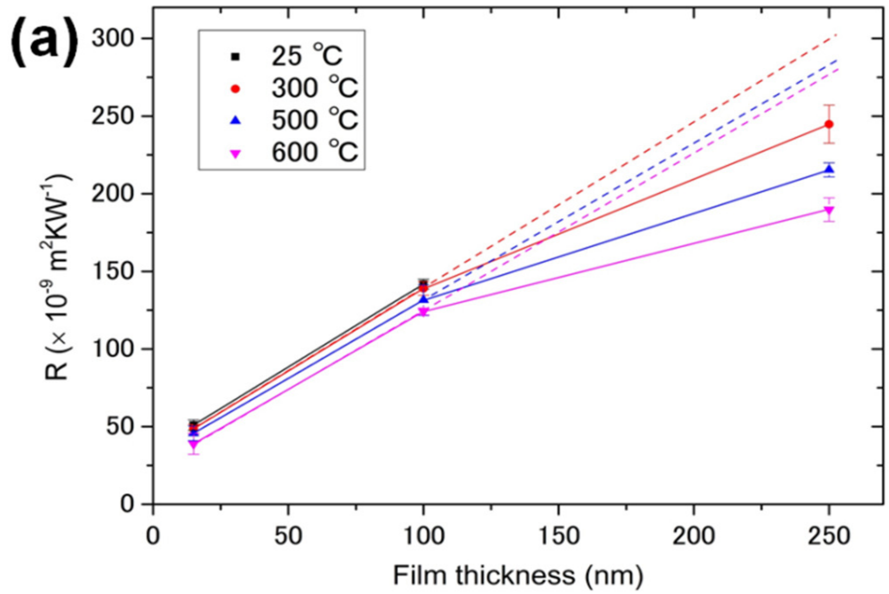




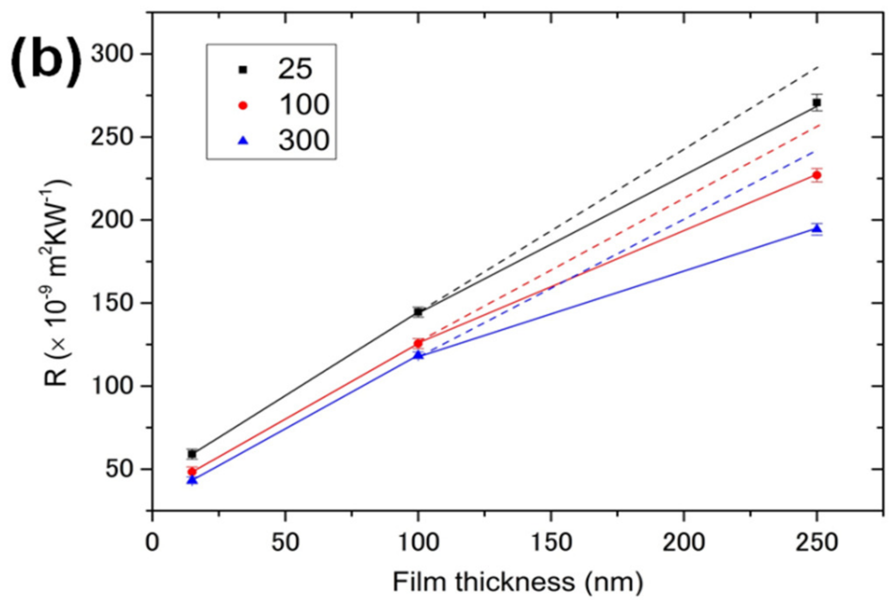
R. Kato, Y. Xu, et. al. , Jpn. J. Appl. Phys, 50, 106602 (2011)

Thermal resistance of amorphous Si(Ge) films as a function of thickness and deposition temperature

Si



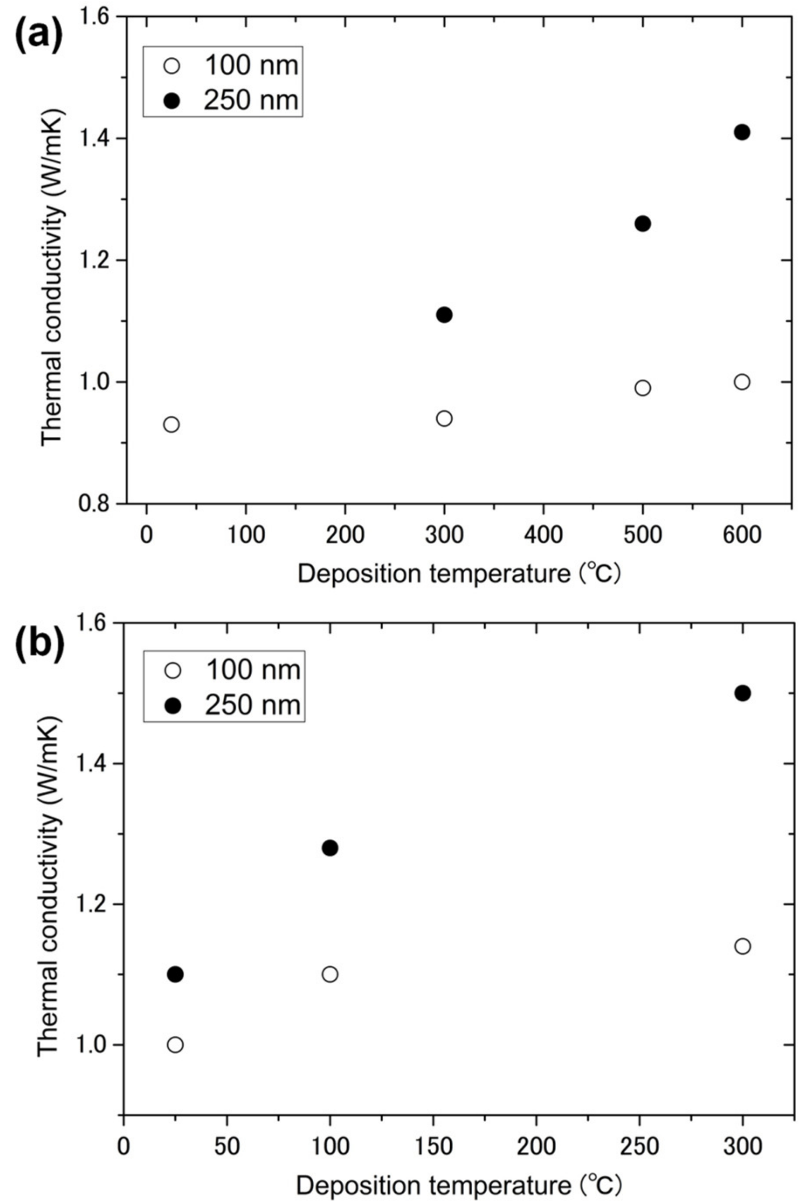
Ge



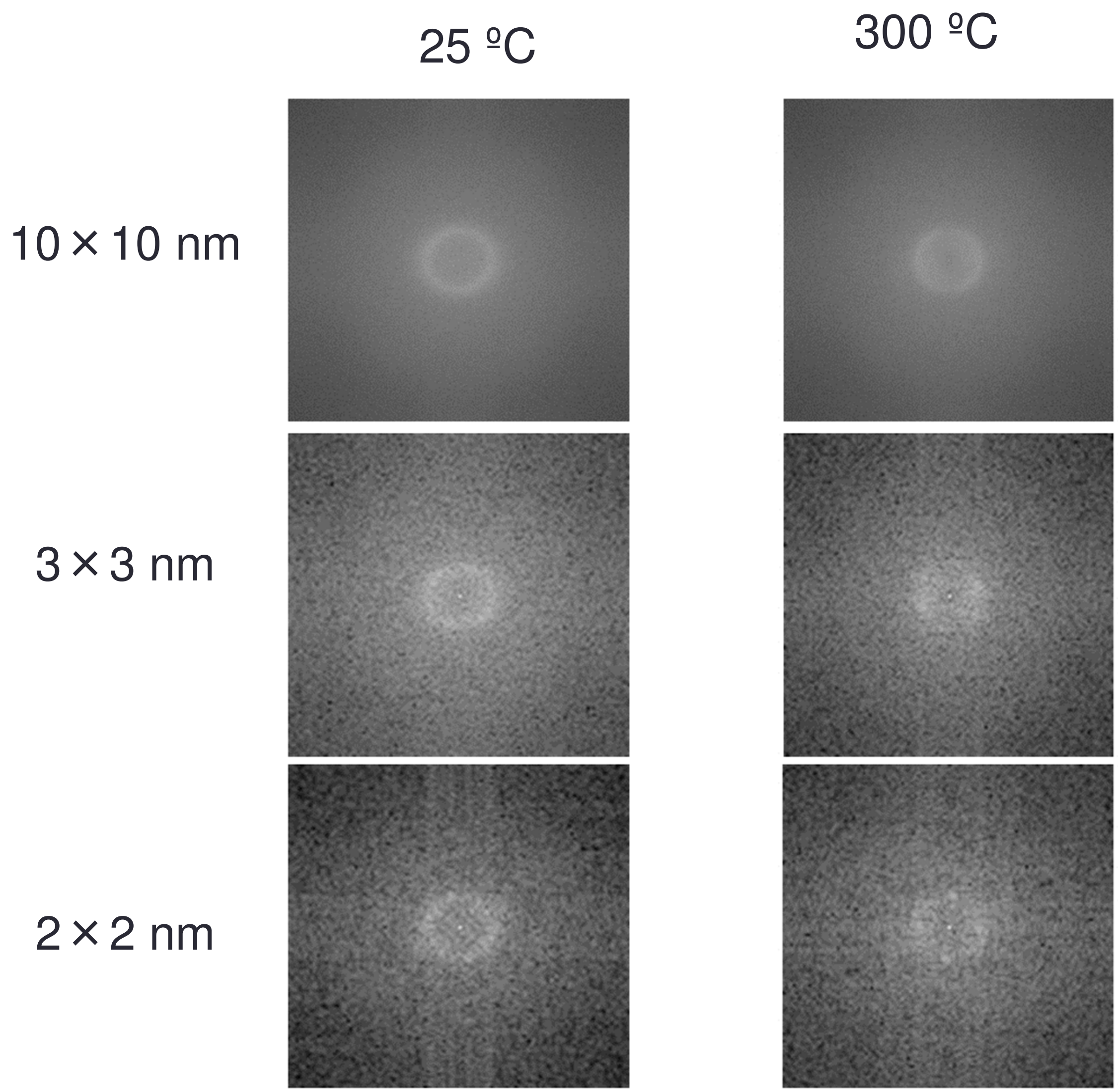
Thermal conductivity of amorphous Si(Ge) film as a function of thickness and deposition temperature

Si

Ge



FFT patterns of different area sizes in Ge films



Conclusion

- Thermal conductivity of amorphous Si and Ge films shows thickness dependence. This result proves that long MFP (>100 nm) phonons exist in amorphous Si and Ge.

- Thermal conductivity of amorphous Si and Ge films shows dependent on deposition temperature. The nano-scaled structural order is supposed to be the responsible for it.