Effect of Phonon Boundary Scattering on Seebeck Coefficient in Silicon Thin Films

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Introduction: Seebeck coefficient S has two components, the diffusive and the phonon-drag part [1]. Recently, Salleh et al. measured S in SOI thin films [2] and found that the film thickness ($t_{\mathrm{Si}} = 9 - 100$ nm) has little impact on the phonon-drag component (see, Fig. 1), which is considered to be proportional to phonon mean free path λ [3]. On the other hand, the experimental observation of the thermal conductivity κ suggests that λ is significantly shortened in ultrathin films by the frequent boundary scattering. Here in our investigation we suspect the effect of specularity in boundary scattering as the cause of this inconsistency.

Method: Specularity in phonon boundary scattering is expressed as $p = \exp(-4\eta^2 k^2)$, where η is the surface roughness RMS and k the phonon wavenumber [4]. Considering the phonons which participate in intravalley electron-phonon scattering in Si, the typical wavenumber of phonons which mainly contribute to the phonon drag can be estimated to be $k_{\mathrm{pd}} \sim 4 \times 10^6$ cm^{-1}. Thus, the value of p relevant to this wavenumber can be obtained from Fig. 2. Then, we calculated λ by considering the phonon scattering mechanisms (Umklapp and normal scattering) as well as the boundary scattering whose relaxation time is expressed as $\tau_B = (L/v)[(1 + p)/(1 - p)]$, where L is the Casimir length and v the sound velocity [5].

Discussion: In Fig. 2 we can see that Si films with $\eta = 0.2$ nm [6] has p of 0.9 at the wavenumber relevant to the phonon-drag contribution. This yields λ to be less affected by the thickness of Si film, as can be seen in Fig. 3. In contrast, phonons which mainly contributes to κ usually has higher wavenumbers ($k_{\mathrm{tc}} \sim 4 \times 10^7$ cm^{-1} @ 300 K [5]), yielding $p \approx 0$ (i.e. diffusive transport) and thus κ is sensitive to changes in film thickness. This difference is thought to be the cause as of why Seebeck coefficient in Si films seemed to be unaffected by the thickness.

Acknowledgement: This work was partially supported by the Murata Science Foundation.

References: [1] M. W. Wu et al., Phys. Rev. B 54, 5438 (1996). [2] F. Salleh et. al., J. Appl. Phys. **105**, 102104 (2014). [3] E. Behnen, J. Appl. Phys. **67**, 287 (1990). [4] J. M. Ziman, *Electrons and Phonons* (Clarendon Press, Oxford, 1960). [5] X. Wang et. al., Sci. Rep. **4**, 6399 (2014). [6] K. Reinhardt et. al. (ed), *Handbook of Silicon Wafer Cleaning Technology, 2nd Ed.* (William Andrew, New York, 2008). [7] T. H. Geballe et al., Phys. Rev. 98, 4 (1955).

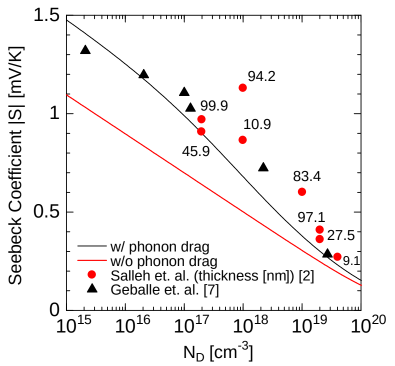

Fig. 1. Seebeck coefficient of Si thin film with various thicknesses (red dots) and bulk silicon (black triangles). Lines shows analytical values for S with phonon-drag (red line), and without phonon-drag (black line). It can be seen that thin films and bulk have similar values of S.

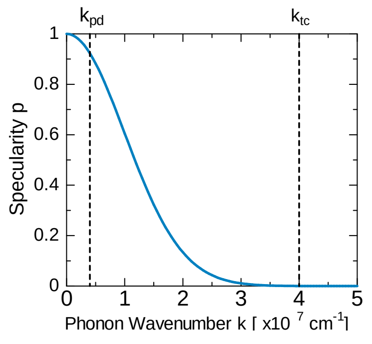

Fig. 2. The estimated specularity of boundary scattering when the surface roughness RMS of $\eta = 0.2$ nm (blue line). Black dashed line shows the typical wavenumber of phonons which contributes in intravalley electron-phonon scattering (k_{pd}) and those contributes in thermal transport (k_{tc}).

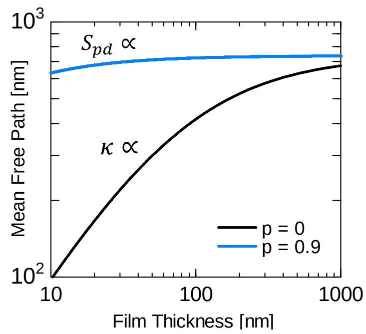

Fig. 3. Mean free path obtained using the specularity value of phonons with wavenumber k_{pd} (see Fig. 2) for $\eta = 0.2$ nm (blue line). Black line shows mean free path when boundary scattering is fully diffusive, which corresponds to (k_{tc}).