Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Estimation of effective electron relaxation times in real thermoelectric materials[1] YUKARI KATSURA[2], The University of Tokyo, National Instutute of Materials Science, KAORU KIMURA, The University of Tokyo — Good samples of thermoelectric materials should be Phonon-Glass-Electron-Crystal (PGEC) [1], which scatters phonons without scattering electrons. However, the actual values of electron relaxation time τ_{el} are not well investigated, and τ_{el} is simply set as 10^{-14} s in many first-principles calculations of thermoelectric properties. In this study, we attempted to estimate the effective values of τ_{el} of various thermoelectric materials, by fitting the calculation results by WIEN2k [2] and BoltzTraP [3] with experimental Seebeck coefficient and electrical conductivity. When we fitted experimental thermoelectric properties of $Si_{0.8}Ge_{0.2}$ samples [4][5], τ_{el}'s at 300 K were 9x10^{-15} s in a highly crystalline sample [4], and 5-6x10^{-15} s in ball-milled polycrystalline samples [5]. Temperature dependences of τ_{el}^{-1} were also different between samples, implying the difference in dominant electron scattering mechanisms. Various samples of thermoelectric materials with fairly high figures of merit exhibited τ_{el} of several 10^{-15} s at 300 K. [1] G. A. Slack, *CRC Handbook of Thermoelectrics*, 407 (1995). [2] P. Blaha, *et al.*, *WIEN2k Users' Guide*, Vienna Univ. of Technology, Austria (2001). [3] G.K.H. Madsen et al., *Comp. Phys. Comm.* 175, 67 (2006). [4] J.P. Dismukes et al., *J. Appl. Phys.* 10 2899 (1976). [5] C.B. Vining et al., *J. Appl. Phys.* 69 4333 (1991).

[1]This work was supported by KAKENHI 16K14379 and the Support Program for Starting up Innovationhub from Japan Science and Technology Agency (JST), Japan.
[2]Name on passport: Yukari Okamoto

Yukari Katsura
The University of Tokyo, National Instutute of Materials Science

Date submitted: 11 Nov 2016 Electronic form version 1.4