Abstract Submitted
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First-principles phonon calculation for Al-(Re,Mn)-Si 1/1-1/1-1/1 approximants N. NAGASAKO, Toyota Central R&D Labs., Inc., R. ASAHI, Toyota Central R&D Labs., Inc., T. TAKEUCHI, Nagoya University — A very low thermal conductivity (∼1 W/Km) and a relatively large Seebeck coefficient in Al-based Mackay-type icosahedral quasicrystal have attracted much interest aiming for thermoelectric applications. We performed first-principles phonon calculations for the Al-(Re,Mn)-Si 1/1-1/1-1/1 approximants [1] to elucidate mechanism of their low thermal conductivity. The total energy and atomic force were calculated for a modeled $Al_{17}(Re,Mn)_4Si_2$ unit cell containing 138 atoms using the projector augmented wave method implemented in VASP code [2], and were then utilized for obtaining a phonon dispersion by the direct method [3]. The calculated lattice specific heat showed very good agreement with experiment, confirming validity of the present calculations. We found localized optical modes with a relatively low frequency (∼2 THz) in the phonon dispersion. We discuss the low thermal conductivity in comparison between the Al-Re-Si and Al-Mn-Si systems via averaged group velocity and umklapp phonon scattering related to these optical modes. [1] Takeuchi et al., Phys. Rev. B70, 144202 (2004). [2] G. Kresse, J. Furthmuller, Phys. Rev. B54, 11169 (1996). [3] MedeA-Phonon, Materials Design, Inc. (2003) based on K. Parlinski, Phonon 3.11 (2002).

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