Development of Novel Multicomponent Chalcogenides

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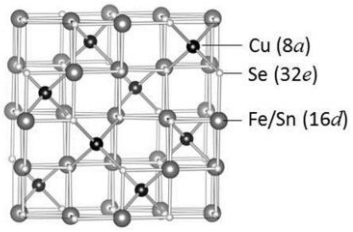
When we search a light-mass thermoelectric (TE) material with intrinsic low lattice thermal conductivity κ_L, we should seek a material with following structural features; (i) numerous atoms in a unit cell and (ii) complex crystal structure, because they lead to a large phonon-phonon scattering probability. [1] In fact, that materials with the structural feature of (ii) exhibit low κ_L below 1 W/Km. [2] The TE material also demands a high power factor of $PF = S^2/\rho$, where S represents thermopower and ρ denotes electrical. The high PF is sometimes realized in a material with a structure belongs to (iii) a high symmetric crystal system wherein the degeneracy of the band extrema N near the Fermi level tend to be large. [1] Therefore, the light-mass materials having the structural feature of (i)-(iii) is expected to show low κ_L, large PF, and high dimensionless figure of merit $ZT = S^2T/\rho(\kappa_L+\kappa_{el})$, where κ_{el} is electronic contribution of thermal conductivity.

We have been focusing multicomponent chalcogenides with a cubic crystal structure, such as quaternary selenospinel $Cu_6Fe_4Sn_{12}Se_{32}$. [3,4] The compound has a Fe/Sn disordered 16*d* crystallographic site which is the cause of structural complexity. As is expected from the structural features, the κ shows low value of 1.2-1.4 W/Km. The ρ decreases and the S increases with increases temperature. Analysis of both properties indicates that the $Cu_6Fe_4Sn_{12}Se_{32}$ behaves as a variable-range hopping (VRH) conductor below 80 K. The ρ exhibits comparatively low value of 10^{-4} Ωm for a VRH conductor and the S reaches large value of 150 μV/K at 300 K, respectively. The results of ρ, S, and Hall coefficient R_H suggest that the low ρ is attributed to the high hole density about 10^{21} /cm^3 and the large S is achieved by heavy hole band and VRH, respectively. The coexistence of comparatively low ρ and large S might be also attributed to the high N due to high symmetry cubic structure.



Crystal structure of selenospinel

Also a pseudo-ternary sulfide with the crystal structure which fulfill the condition of (i)-(iii) have been studying. The TE properties will be presented.

[1] F. J. DiSalvo, Science **285**, 703 (1999).
[2] G. J. Snyder and E. S. Toberer, Nature mater. **7**, 105 (2008).
[3] K. Suekuni *et al*., J. Appl. Phys. **109**, 083709 (2011).
[4] K. Suekuni *et al*., J. Electron. Mater., in print.