Theoretical acanthite-like model for the solid-liquid structure of Cu_2S: electronic and transport properties

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Abstract:

Cu_2S has long been studied for its potential applications in the field of photovoltaic solar cells and, most recently, thermoelectricity (TE). The interesting properties of this material are mainly driven by the liquid-like behavior of the Cu atoms, which is also a barrier that confuses us in determining their atomic positions and electronic properties. In this work,[1] using a theoretical model driven from a similar low-temperature phase of Ag_2S called the acanthite-like phase,[2] we confirm the appearance of an electronic structure with an indirect bandgap of 0.9-0.95 eV as observed experimentally before. The formation of point defects and their influence on the conductive properties of Cu_2S are also discussed. According to the bonding analysis and formation energy aspect, Cu vacancy is the most preferred defect to form in Cu_2S, which primarily affects the conductive behavior as a p-type semiconductor. Finally, the use of the electron-phonon scattering approximation allows us to estimate the electron energy relaxation time, reproducing the reasonable results of transport property compared to experimental observation. Therefore, demonstrating that the acanthite-like model is ideally suitable and can be used for the computational design of TE materials related to the low-temperature phase of Cu_2S.

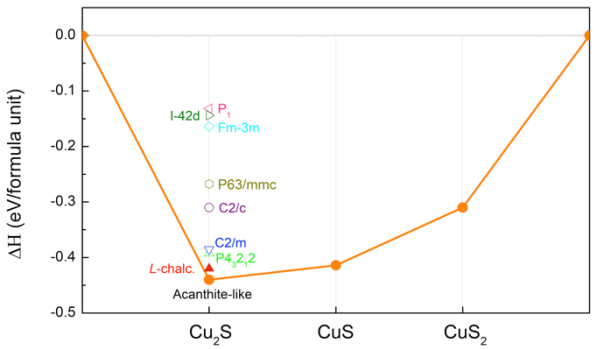

Fig.1: Formation enthalpy of several structures at the stoichiometric limit of Cu-S system, indicating the stability of the acanthite-like model.

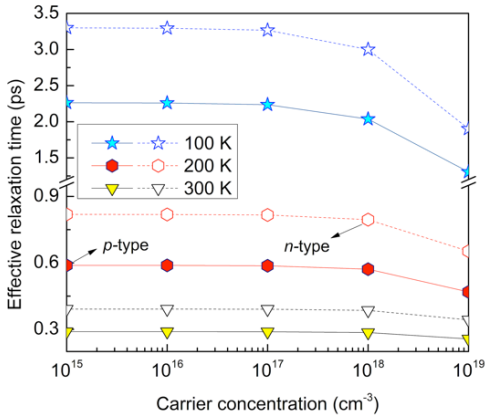

Fig.2: The electron energy relaxation time as a function of doping concentrations predicted by electron-phonon average approximation.

[1]H. N. Nam, K. Suzuki, T. Q. Nguyen, A. Masago, H. Shinya, T. Fukushima, and K. Sato, arXiv:2110.09117 (2021).
[2]H. N. Nam, R. Yamada, H. Okumura, T. Q. Nguyen, K. Suzuki, H. Shinya, A. Masago, T. Fukushima, and K. Sato, Phys. Chem. Chem. Phys. 23, 9773 (2021).