

Molecular-Dynamics Simulations of Copper Diffusion in Copper Chalcogenides

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It was recently discovered that copper chalcogenides Cu_2S and Cu_2Se are viable candidates for thermoelectric materials with high figure of merit (ZT) values at temperatures around 1,000 K [1,2]. And the possible reason for the high ZT is the low thermal conductivity arising from liquid-like Cu atoms in those phases. In this work, we perform first-principles molecular dynamics simulations to study the motion of Cu atoms in the high-temperature phases of Cu_2S and Cu_2Se and confirm the liquid nature of Cu atoms. To get a better understanding of the diffusion patterns of the systems, we have examined different phases of Cu_2S (hexagonal and cubic phases with increasing temperature). Starting from the hexagonal phase the Cu atoms show a disordered/liquid-like feature with a jump diffusion pattern. We find that the diffusion is faster in the x-y directions than in the z direction. A more isotropic diffusion pattern is found for the high-temperature cubic phase with a much larger diffusion coefficient.

[1] Y. He et al. *Adv. Mater.* 26, 3974 (2014)

[2] H. L. Liu et al. *Nat. Mater.* 11, 422 (2012)