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Effect of lattice relaxation on thermal conductivity prediction via molecular dynamics simulations: study on fcc-based structures[1] MIN YOUNG HA, WON BO LEE[2], Seoul Natl Univ — This work studies the computational details of molecular dynamics (MD) thermal conductivity prediction with Green-Kubo method. Little consensus has been made among researchers about the choice of lattice parameter in MD thermal conductivity calculation, leading to mutually disagreeing reports. Simulations on fcc-based structures with different lattice parameters were performed to calculate lattice thermal conductivities, heat current autocorrelation functions, and phonon density of states. The results were compared to experimental reports and ab initio calculations to conclude that lattice volume relaxation in isobaric-isothermal (NpT) ensemble is crucial for accurate prediction of thermal conductivity. In addition, effect of domain size and interatomic potential cutoff distance was also studied in the context of lattice relaxation, and it was verified that conventional choice of cutoff distance may result in underestimation of thermal conductivity. After analyzing the size and cutoff dependence of lattice parameter, a new criterion for cutoff distance was suggested. Simulations were performed with the newly developed simulation parameters, and showed improved agreement with experimental and ab initio results.

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