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Anharmonicity Rise the Thermal Conductivity in Amorphous Silicon[1] WEI LV, ASEGUN HENRY, Georgia Institute of Technology — We recently proposed a new method called Direct Green-Kubo Modal Analysis (GKMA) method, which has been shown to calculate the thermal conductivity (TC) of several amorphous materials accurately. A-F method has been widely used for amorphous materials. However, researchers have found out that it failed on several different materials. The missing component of A-F method is the harmonic approximation and considering only the interactions of modes with similar frequencies, which neglect interactions of modes with large frequency difference. On the contrary, GKMA method, which is based on molecular dynamics, intrinsically includes all types of phonon interactions. In GKMA method, each mode's TC comes from both mode self-correlations (autocorrelations) and mode-mode correlations (crosscorrelations). We have demonstrated that the GKMA predicted TC of a-Si from Tersoff potential is in excellent agreement with one of experimental results. In this work, we will present the GKMA applications on a-Si using multiple potentials and gives us more insight of the effect of anharmonicity on the TC of amorphous silicon.

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