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Role of non-adiabatic carrier dynamics in non-thermal phase transition of Ge-Sb-Te alloy JUNHYEOK BANG, Korea Basic Science Institute (KBSI), YIYANG SUN, X.-Q. LIU, Rensselaer Polytechnic Institute (RPI), F. GAO, University of Michigan, S. B. ZHANG, Rensselaer Polytechnic Institute (RPI)
— Non-thermal phase transition driven by femtosecond laser irradiation has been explained by the simple static plasma annealing effect: excitation of a large fraction of valence electrons to conduction bands weakens lattices and leads to the structural phase transition in low temperature. Here, by time-dependent density functional theory and molecular dynamics study of Ge-Sb-Te alloys, we find that the energy-dependent dynamics of excited carriers is critical in determining the phase transition mechanism. For low energy carriers electron-phonon scattering becomes a dominant relaxation process, and for high energy carriers electron-electron scattering remains a dominant relaxation process. As a result, we observe significant ionic temperature increase for low energy excitation, which aids phase transition by thermal effect, and non-thermal phase transition for high energy excitation. This provides a new conceptual framework in understanding fundamental phenomenon of the phase transition.

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