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Simulations of Photo-induced Nonequilibrium Dynamics in Charge Density Wave Materials LINGHUA ZHU, New Jersey Institute of Technology, TSEZAR F. SEMAN, MICHEL VAN VEENENDAAL, Northern Illinois University and Argonne National Laboratory, KEN AHN, New Jersey Institute of Technology — We present the results of our simulations for nonequilibrium dynamic of lattice distortion and electronics state in charge density wave materials initiated by optical pulses. We use a two-dimensional AB_2 square lattice as a model for the charge density wave systems. The coherent dynamics of B ions is considered through the Newtonian equation. The dynamics of electron distribution on A sites due to scattering with other electrons and incoherent phonons is described through the Boltzmann equation. The effect of optical pump is modeled as electron excitations in the initial state. We analyze the coupled dynamics of charge density wave order parameter, coherent lattice distortions and electronic state in photo-induced non-equilibrium states through computational simulations and compare with recent experimental results.

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