

Abstract Submitted
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Ultrafast Photoinduced Structural Dynamics in Graphite¹

ZHIBIN LIN, ROLAND ALLEN, Department of Physics, Texas A&M University — In this work, we employ the density-functional-based tight-binding approach of Frauenheim and coworkers in simulations employing semiclassical electron-radiation-ion dynamics (SERID), which treats the coupled dynamics of electrons and ions during the nonadiabatic processes induced by laser irradiation. A series of computer simulations are performed in studies of graphite responding to femtosecond-scale laser pulses of various intensities and durations. It is found that the contraction of the interlayer distance in graphite happens shortly after optical excitation. Transient changes in the interlayer distance are related to changes in the interlayer bonding due to ultrafast changes in the populations of the electronic states. Results of these computational studies are compared with recent pump-probe experimental data on graphite.

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