Abstract Submitted
for the 4CF09 Meeting of
The American Physical Society

Ultrafast Laser-induced Structural and Electron Dynamics in Graphite ZHIBIN LIN, REMRSEC and Dept. of Physics, Colorado School of Mines, ROLAND ALLEN, Dept. of Physics, Texas A&M Univ. — Ultrafast structural and electron dynamics in graphite under femtosecond (fs) laser irradiation are investigated in density-functional-based simulations. We show from our simulations that it is possible to separate a graphene mono-layer from graphite surface at moderate laser excitation where no melting occurs. Strong vibrational excitation of graphene layers is found to cause this monolayer separation. At higher laser excitation, covalent bonds between carbon atoms are significantly weakened by the presence of a large number of excited electrons leading to an ultrafast melting within a few tens of fs following the laser irradiation. In addition, we have observed a potentially useful phenomenon from our dynamic simulations: the excited electrons automatically equilibrate to a Fermi-Dirac distribution within 100 fs, solely because of their coupling to the ionic motion, even though the resulting electronic temperature is one to two orders of magnitude higher than the kinetic temperature defined by the ionic motion. Microscopic simulations like these can then provide the separate electronic and kinetic ionic temperatures, chemical potentials, pressures, and non-hydrostatic stresses as input for studies on larger length and time scales.

Zhibin Lin
REMRSEC and Dept. of Physics, Colorado School of Mines

Date submitted: 28 Sep 2009 Electronic form version 1.4