8th. World Congress on Computational Mechanics (WCCM8)
5th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 –July 5, 2008
Venice, Italy

Enhanced Molecular Dynamics for Simulating Thermal and Charge Transport Phenomena

*** Reese E. Jones[1], Jeremy A. Templeton[1], Greg J. Wagner[1], David Olmsted[2], and Normand A. Modine[2]**

[1] Sandia National Laboratories
Livermore, CA 94551 USA
rjones@sandia.gov
jatempl@sandia.gov
gjwagne@sandia.gov

[2] Sandia National Laboratories
Albuquerque, NM 87185 USA
dolmste@sandia.gov
namodin@sandia.gov

Key Words: *atom-continuum coupling, molecular dynamics, finite elements, two temperature model.*

ABSTRACT

In modeling non-equilibrium thermal transport in solids, classical molecular dynamics (MD) has the primary strength of explicit representation of phonons and defects that scatter phonons. On the other hand, electrons and their role in thermal transport are missing. These effects are vital in applications ranging from laser processing of materials to thermal transport in conducting nanotubes and nanowires. Predictive models of the phenomenology of the interactions between the charge carriers and the "atoms" represented in MD exist. For instance, the so-called "two temperature" model (TTM) [1, 2] has been applied on the continuum level to simulate the rapid exchange of thermal energy between electrons and phonons in a conductor. The two temperature model, which is derived from the Boltzmann transport equation, is simply a split of the balance of energy into the energy transmitted via electrons and that transmitted via phonons

$$\rho_e c_e \dot{\theta}_e = \boldsymbol{\nabla} \cdot (\mathbf{k}_e \boldsymbol{\nabla} \theta_e) - q_{\text{e-p}}(\theta_e - \theta_p)$$
$$\rho_p c_p \dot{\theta}_p = \boldsymbol{\nabla} \cdot (\mathbf{k}_p \boldsymbol{\nabla} \theta_p) + q_{\text{e-p}}(\theta_e - \theta_p)$$

with diffusive and exchange terms.

Taking the TTM as a framework for coupling and following [3, 4], we represent the phonon system with MD and the electron system with finite elements (FE). Figure 1 shows the configuration of an example simulation where an initial Gaussian temperature profile is prescribed for the electron temperature mimicking heating with a laser pulse. This temperature field interacts with an initially uniform phonon temperature field partially represented on the MD lattice and the FE mesh (where no atoms are present). Figure 2 shows that the two systems come to a common average temperature and that that the temperatures in the two systems become more uniform over time. Interestingly, Figure 2 also shows the transition of the dominant transfer mechanism from fast electron-mediated diffusion to slower electron-phonon exchange.

By coupling classical MD to FE based models of the missing physics, we enable the simulation of a broad range of physical phenomena from the rapid exchange of heat between the electron and phonon

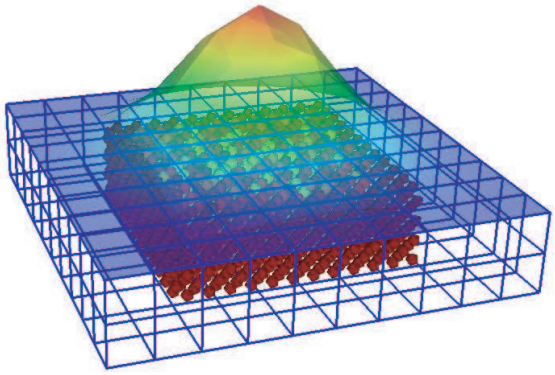

Figure 1: Configuration of the FE mesh and MD lattice

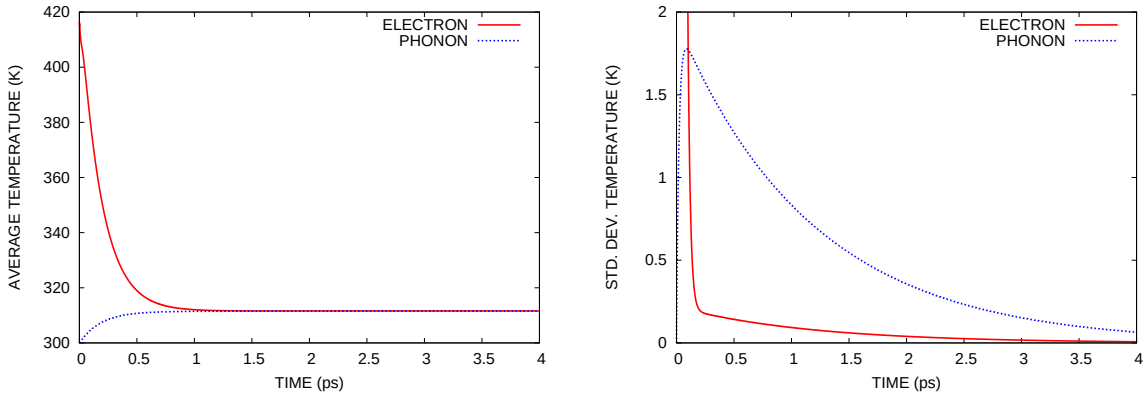

Figure 2: Temperature evolution

carriers in a lattice through current induced thermal failure of nanowires. This approach is intrinsically multiscale and multiphysics, due to the tight coupling between the MD and FE paradigms, and utilizes the inherent strengths of each.

References

[1] M. I. Kaganov, I. M. Lifshits, and L. V. Tanatarov. Relaxation between electrons and the crystal lattice. *Zhurnal Eksperimental'noi i Teoreticheskoi Fiziki*, 31(2(8)):232 – 237, 1956.

[2] L. Jiang and H. L. Tsai. Improved two-temperature model and its application in ultrashort laser heating of metal films. *Journal of Heat Transfer*, 127(10):1167 – 1173, 2005.

[3] D. S. Ivanov and L. V. Zhigilei. Combined atomistic-continuum modeling of short-pulse laser melting and disintegration of metal films. *Physical Review B*, 68(6):064114 –, 2003.

[4] D. S. Ivanov and L. V. Zhigilei. Combined atomistic-continuum model for simulation of laser interaction with metals: Application in the calculation of melting thresholds in Ni targets of varying thickness. *Applied Physics A: Materials Science and Processing*, 79(4-6):977 – 981, 2004.