MOLECULAR DYNAMICS SIMULATIONS OF SHOCKS INCLUDING ELECTRONIC HEAT CONDUCTION AND ELECTRON-PHONON COUPLING

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Abstract. Shocks are often simulated using the classical molecular dynamics (MD) method in which the electrons are not included explicitly and the interatomic interaction is described by an effective potential. As a result, the fast electronic heat conduction in metals and the coupling between the lattice vibrations and the electronic degrees of freedom can not be represented. Under conditions of steep temperature gradients that can form near the shock front, however, the electronic heat conduction can play an important part in redistribution of the thermal energy in the shocked target. We present the first atomistic simulation of a shock propagation including the electronic heat conduction and electron-phonon coupling. The computational model is based on the two-temperature model (TTM) that describes the time evolution of the lattice and electron temperatures by two coupled non-linear differential equations. In the combined TTM-MD method, MD substitutes the TTM equation for the lattice temperature. Simulations are performed with both MD and TTM-MD models for an EAM Al target shocked at 300 kbar. The target includes a tilt grain boundary, which provides a region where shock heating is more pronounced and, therefore, the effect of the electronic heat conduction is expected to be more important. We find that the differences between the predictions of the MD and TTM-MD simulations are significantly smaller as compared to the hydrodynamics calculations performed at similar conditions with and without electronic heat conduction.

INTRODUCTION

Molecular Dynamics (MD) has been intensively used to study ultrafast non-equilibrium phenomena in solids. In particular, MD has been proved to be an efficient tool for the microscopic analysis of shock waves [1]. Simulations up to date have dealt mostly with single crystal samples, which are in general far from the experimental "single crystals" and polycrystalline samples. Grain boundaries (GB) form one of the relevant groups of defects to be considered. MD simulations have suggested that GB can melt at lower temperature as compared to the bulk material [2], possibly leading to a decreased yield stress. This could explain recent experimental results on Rayleigh-Taylor (RT) instability growth in a polycrystalline Al [3]. MD simulations of shocks in fluids have been related to predictions by hydrodynamic (HD) calculations [4]. Recent HD simulations of shock wave heating of a GB region, Fig. 1, show large differences (~2000 K at the GB) in the temperature profiles obtained with and without electronic heat conduction. In the HD simulation illustrated by Fig. 1, zones corresponding to the GB were described by the same equation of state (EOS) as the bulk Al with an initial/equilibrium density decreased to 0.75 of the bulk density. Note that the results of HD calculations may no longer be valid at small spatial scales, such as the thickness of a GB. Therefore, the thickness of the GB region in the HD simulation was chosen to be 10 nm, several times larger that an effective thickness of a typical GB. These rough approximations were intended to

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provide some initial feedback into possible GB evolution scenarios under shocks. In these simulations, fast electron conduction led to significant energy dissipation from the GB region.

MD simulations can be used to simulate a more realistic GB, without any pre-existing assumptions on the EOS, density, or thickness of the GB. The electronic heat conduction, however, cannot be reproduced within a classical MD model, which only includes the lattice contribution to the heat conduction. Since the electronic contribution to the thermal conductivity of a metal is orders of magnitude larger than the lattice contribution, conventional MD significantly underestimates the total thermal conductivity in metals. In order to overcome this limitation we combine MD with a continuum description of the electronic heat conduction, as briefly described below.

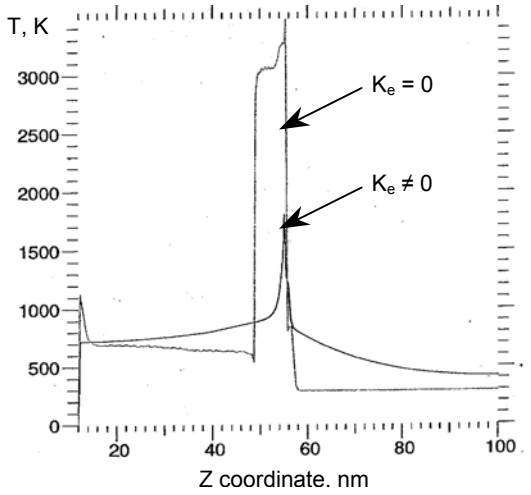

Figure 1. Temperature profiles obtained in HD simulations of a shock traversing a grain boundary, with and without electronic heat conduction.

THE COMBINED TTM-MD MODEL

A hybrid computational model that combines the classical MD method for simulation of fast non-equilibrium processes in the shocked material with a continuum description of the electronic heat conduction is used in the simulations. The model is based on the so-called two temperature model (TTM) [5], that describes the time evolution of the lattice and electron temperatures by two coupled non-linear differential equations. The TTM was originally developed for strong electron-phonon non-equilibrium due to the fast electronic excitation. The model, however, is also appropriate for situations where the electron and lattice temperatures are close to each other and, in particular, is applicable for the description of the electronic heat conduction in a material undergoing shock wave heating. In the combined TTM-MD method [6-8], the MD completely substitutes the TTM equation for the lattice temperature. The diffusion equation for the electron temperature is solved by a finite difference method simultaneously with MD integration of the equations of motion of atoms. The electron temperature enters a coupling term that is added to the MD equations of motion to account for the energy exchange between the electrons and the lattice. A modified, as compared to earlier works [6,7], formulation of the coupling term is used in the model. The new formulation [8] distinguishes between the thermal velocities of the atoms and the velocities of their collective motion. It also does not require *a priori* knowledge of the lattice heat capacity of the model system, which is, in general, a function of temperature. The expansion and density variations, predicted in the MD part of the model, are accounted for in the continuum part of the model. A complete description of the combined TTM-MD model is given elsewhere [8]. In this paper, we report the results of MD and TTM-MD simulations of shock wave heating of a tilt GB in an Al bi-crystal. The effect of the electronic heat conduction on the temperature evolution in the GB region is discussed based on the simulation results.

The simulations reported in this article are performed for a 300 kbar shock wave propagating through an Al bi-crystal containing a (110) $\sum 5$ tilt boundary. The initial MD system is an FCC bi-crystal with dimensions 9.17 × 12.3 × 21.8 nm, periodic boundary conditions in the directions parallel to the shock front, and a grain boundary located in the middle of the computational cell. Inter-atomic interaction is described by the embedded-atom method (EAM) in the form and parameterization suggested in [9]. Before applying the shock loading, the system is equilibrated at 300 K and zero pressure. The parameters used in the TTM equation for the electronic temperature are given in [10].

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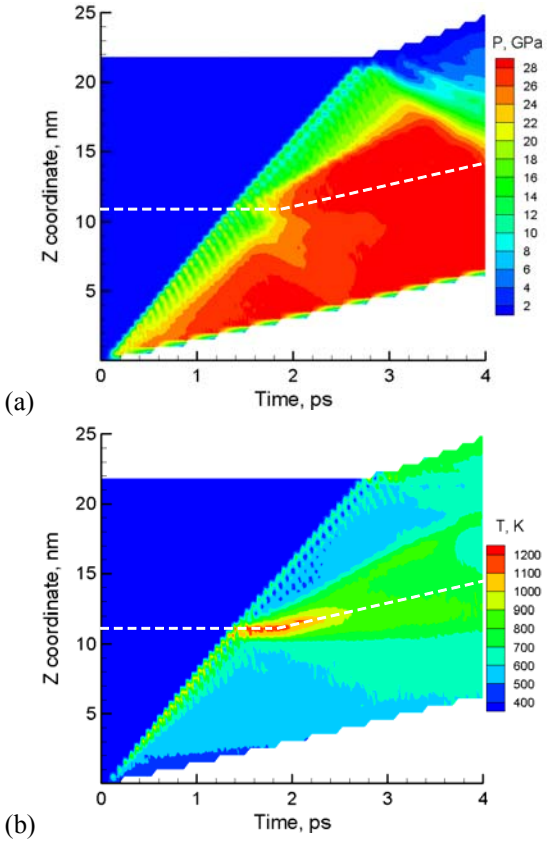

Figure 2. Pressure (a) and temperature (b) contour plots for a TTM-MD simulation of a 300 kbar shock in an Al sample with a tilt GB. The location of the GB is indicated by the dashed line.

In the combined TTM-MD model the cells in the finite difference discretization are related to the corresponding volumes of the MD system. The local lattice temperature and pressure are defined for each cell from the average kinetic energy of the thermal motion of atoms and through the virial equation, respectively.

The shock wave is generated by applying additional forces to a layer of atoms that make up a "piston" located on one side of the MD computational cell. The forces are chosen so that a constant pressure of 300 kbar is maintained in a region adjacent to the piston. In the following section, we present and compare results obtained in simulations performed with and without the electron conduction included.

RESULTS AND DISCUSSION

Both MD and TTM-MD simulations are run for four picoseconds so that the shock wave has enough time to reach the back surface but the reflected wave does not reach the GB. The temperature and pressure contour plots are shown in Fig. 2 for the TTM-MD simulation performed with the electron heat conduction included. In the pressure plot we can see a partial reflection of the shock (v_{shock}~7.5 km/s) from the GB at ~1.5 ps, and a complete reflection of the shock wave from the back surface of the computational cell at ~3 ps. After the shock reaches the GB, we can see that the GB starts to move with the piston velocity, as expected. In the temperature contour plot we can see that the interaction of the shock wave with the GB leads to a transient thermal spike in the GB region. A very similar temperature and pressure distributions are observed in MD simulations without the electron heat conduction. We observe only small differences in temperature distributions between the two simulations, whereas there is practically no difference in the pressure plots.

The difference in temperature observed in the GB region is ~50-200 K at t~1.6-2.6 ps ps. Therefore, the effect of the electronic heat conduction is relatively small. It can only play a significant role when the maximum local temperature reached at the GB is close to the melting point. In this case the electronic heat conduction may prevent melting in a system that would otherwise melt in a pure MD simulation.

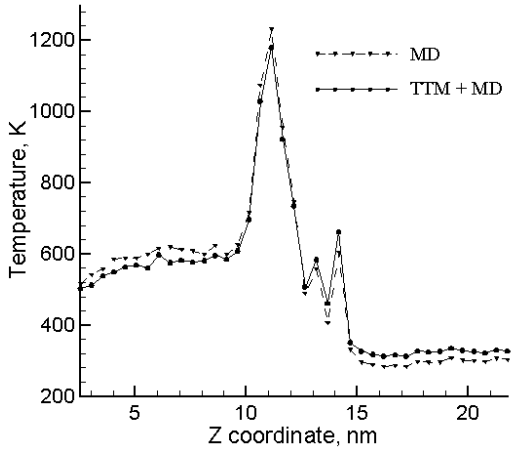

Figure 3. Temperature profiles for the MD and TTM-MD simulations at t = 1.8 ps.

The fast electronic heat conduction leads to the increasing temperature ahead of the shock wave and decreasing temperature behind the shock front in the TTM-MD simulation as compared to the MD simulation, Fig. 3.

The atomic-level picture of the structural changes induced by the shock wave can be seen in Fig. 4. The (110) Σ5 tilt boundary is initially located at Z~12 nm. At t=2.0 ps, a slab of material with a tilt several degrees smaller than the original one appears in a region adjacent to the grain boundary, Z~12-13 nm. By 2.8 ps this region has grown thicker, Z~13-16 nm, giving a velocity of growth of ~2.5 km/s ~ $v_{shock}/3$. The train of elastic precursors can be seen well ahead of the upper boundary for this region. No plastic front formation is observed at this shock pressure for a perfect crystal. This GB "splitting" appears in both MD and TTM-MD simulations. A more detailed study of this effect is in progress.

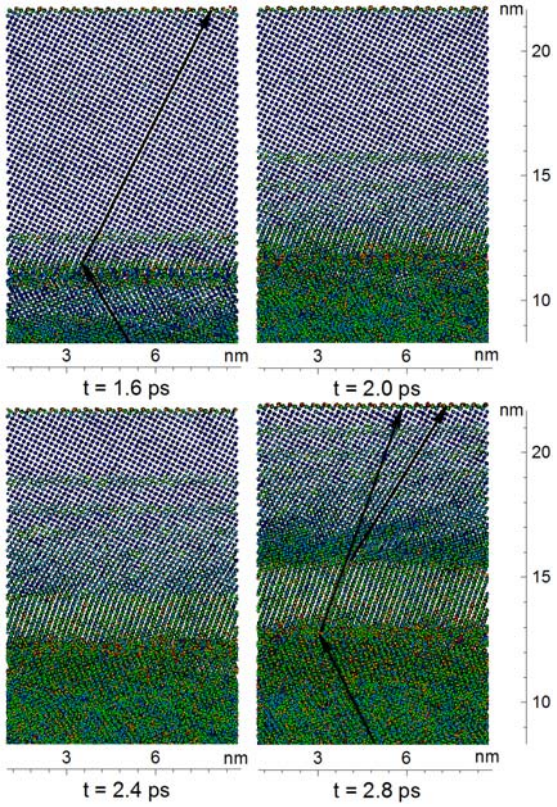

Figure 4. Grain boundary "splitting" for a 300 kbar shock. Crystal orientation is indicated by arrows.

SUMMARY

Simulations of a 300 kbar shock wave propagation in an Al target containing a single (110) ∑5 tilt grain boundary are performed with (TTM-MD) and without (MD) electronic heat conduction. We find that the differences between the predictions of the MD and TTM-MD simulations are relatively small. The difference in the lattice temperatures at the GB was ~50-200 K at t~1.6-2.6 ps. A significantly stronger effect of the electronic heat conduction is predicted in the HD calculations

A "splitting" of the initial GB is observed in both the MD and TTM-MD simulations. The mechanism of the formation of the second tilt GB is being further investigated. Additional studies including other ordered and disordered boundaries, at several shock pressures, are also needed to evaluate the change in the mechanical properties of the shocked grain boundary, which would be important to estimate its influence on the RT growth [3]. The TTM-MD model will be also used to investigate the role of the electronic heat conduction and the strength of the electron phonon coupling in plastic deformation and melting induced by strong shocks.

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