Lattice dynamics and solid-state plasticity experiments at high pressures and strain rates

Bruce A. Remington

Lawrence Livermore National Laboratory

Experiments are being developed on high power lasers and intense x-ray sources, such as the Omega laser at LLE, the Janus and NIF lasers at LLNL, and LCLS at SLAC to study lattice dynamics and solid-state plasticity at high pressures and strain rates. These experiments probe the plastic response of materials to high pressure (50-500 GPa), high strain rate ($10^6 - 10^{10}$ s^{-1}) deformation. Three classes of experiments in tantalum, a model bcc metal, will be described. Dynamic diffraction experiments with a time resolution of ~0.1 ns or shorter are being developed to probe the microscopic lattice response of samples to a strong shock. [1,2] In particular, the time scale for the onset of plasticity and the rate of the 1D to 3D lattice relaxation are a direct measure of how rapidly dislocations can be generated and transported on sub-nanosecond time scales. [3] Macroscopic plastic flows at high pressure and strain rate can be generated that span a few tens of nanoseconds by using the Rayleigh-Taylor or Richtmyer-Meshkov fluid instabilities. [4,5] Finally, shock driven samples are also recovered so that the residual microstructure caused by the shock and subsequent plastic flow can be examined by SEM, TEM, and other laboratory techniques. [6,7] Results from all three classes of experiments will be compared with simulations using various models of flow stress, and a multi-scale model for bcc strength. [8,9] The mechanisms for plastic deformation and flow vary, depending on the sample pressure, temperature, and strain rate due to the shock or ramp compression. Given the small sample sizes and short time scales of the experiments, MD simulations also provide a valuable guide to the lattice level dynamics, and exhibit significant sensitivity in the predicted results to the interatomic potential. [10,11] Results from the three classes of experiments summarized above will be described, comparisons to theory and simulations given, and a path forward suggested.

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Grain boundary dynamics from atomistic simulations

C. Brandl[1], D. Perez[2], T. C Germann[2]

[1]Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-WBM), Karlsruhe, Germany
[2]Los Alamos National Laboratory, Theoretical Division, Los Alamos, USA

The motion of grain boundaries is crucial for the evolution of microstructure both in processing and in application. In experiments, the grain boundary motion is usually studied at relatively high homologous temperature during long times under small mechanical loads. But grain boundary motion is also shown to be a deformation mechanism occurring at high stresses and relative low temperatures, as for example in deformation studies of nanocrystalline metals and shock loading. Using molecular dynamics simulations and transition search methods (string method), the interface motion of grain boundaries is used to elucidate the role of atomistic structure (morphology) and velocity-driving force relation (mobility) for two different driving force mechanisms: elastic anisotropy and shear coupled motion.

As function of temperature and driving force, the grain boundary mobility shows a complex nonlinear behavior beyond the conventional conjecture of Arrhenius-like temperature-dependence in mobility and linear velocity-driving force relation. The velocity-limiting mechanisms range from the pinning-depinning transition at low temperature, through rare-event dynamics of critical “kink- pair” disconnection nucleation along intrinsic grain boundary dislocations, to fluctuating randomly diffusive grain boundary motion at low driving forces and high temperatures. The interfaces’ dynamics are discussed in context of previous atomistic studies and necessary ingredients for a mesoscale model of GB motion.

Experimental investigation of metals at high strain rates

Jonathan C. Crowhurst, Michael R. Armstrong, Bryan W. Reed, Joseph M. Zaug, Harry B. Radousky, Damian C. Swift, Roger W. Minich, Nick E. Teslich, Mukul Kumar

Lawrence Livermore National Laboratory, Livermore, California 94550, USA

Materials at extreme strains and strain rates continue to present both formidable theoretical and experimental challenges. Shock compressed solids are a particularly relevant example. Shock waves have been used for many years to obtain, on the basis of fundamental conservation laws, highly precise material-specific relationships between volume and pressure. However, the detailed physics of shock waves, at even fairly low stresses, and in simple metals, is still imperfectly understood. This has motivated our efforts to characterize the behavior of various metals under high strain rates and to make comparisons to previous results established at lower strain rates, as well as to recent theoretical results.

In this this presentation, we will discuss our measurements on aluminum, iron and tantalum thin films. To obtain these data we have used a table-top scale laser to drive shock waves in polycrystalline samples of thicknesses of ~ 1 μm, combined with an ultrafast interferometer to measure free surface histories with a time resolution of ~ 10 ps. For aluminum [1], we will compare our assumed steady wave data at strain rates of up to 10^{10} s^{-1} to literature data up to ~ 10^{7} s^{-1} and show that the well-known fourth power scaling relation of strain rate to shock stress is maintained even at these very high strain rates. For iron [2], we will show that at strain rates of ~ 10^{9} s^{-1}: 1. The $\alpha \rightarrow \epsilon$ transition begins very soon (within ~ 100 ps) after the arrival of a large elastic precursor and is essentially complete within a similar time period thereafter. 2. The deviatoric stress before the transition begins can exceed 3 GPa. 3. The majority of the material transforms at stresses up to ~25 GPa, or nearly twice as large as inferred in longer time scale experiments; and, 4., the separate P1 and P2 waves seen at lower strain rates are not observed. We will also discuss our recent results obtained from tantalum thin films and how they compare with those obtained on other shock wave platforms.

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Temperature and high strain rate dependence of tensile deformation behavior in single crystal iron from dislocation dynamics simulations

Meijie Tang, Jaime Marian

Lawrence Livermore National Laboratory, Livermore, California 94550, USA

We conduct dislocation dynamics (DD) simulations of Fe periodic single crystals under tensile load at several high strain rates and temperatures. The simulations are connected to the atomistic scale via recently-calculated, temperature-dependent dislocation mobility relations. We explore strain rates from 10^4 to 10^6 s^{-1} at temperatures of 100, 300, and 600 K. We compute the flow stress as a function of strain rate and temperature and find very good agreement with experimental data for Fe, suggesting that strain hardening is the dominant materials response mechanism in the range of conditions explored here.

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Multiscale modeling of high-rate plastic deformation of polycrystalline bcc metals

Robert E. Rudd[1], A. Arsenlis[1], N. R. Barton[1], R. M. Cavallo[1], A. J. Comley[2], B. R. Maddox[1], H.-S. Park[1], C. Plechaty[1], S. T. Prisbrey[1], C. E. Wehrenberg[1], B. A. Remington[1]

[1]Lawrence Livermore National Laboratory, Livermore, California 94550, USA
[2]AWE, Aldermaston, Reading RG7 4PR United Kingdom

Multiscale strength models for high-rate deformation have been developed for tantalum and vanadium starting with atomic bonding and extending up through the mobility of individual dislocations, the evolution of dislocation networks and so on until the ultimate material response at the scale of an experiment. [1] These models are based on an information-passing, hierarchical strategy starting with density functional theory, and going through classical molecular dynamics and dislocation dynamics to produce a constitutive model well suited for use in finite element and other continuum simulations. In parallel with the development of the multiscale strength models, high-rate plastic deformation has been the subject of increasing experimental activity. High energy laser platforms such as the National Ignition Facility offer the possibility to study plasticity at extremely high rates in shock waves and, importantly, in largely shock-free ramp-compression waves. [2] Experiments have been conducted on tantalum and vanadium at pressures of ~100 GPa and strain rates of ~10^7/s. [3] In-situ x-ray diffraction also can provide information about the shear stress in a metal undergoing rapid deformation. These experiments have been conducted on Ta also at pressures of ~100 GPa. [4] Remarkably, the predictions of the multiscale model agree well with the experiments without adjustable parameters. Here we review the construction of a multiscale strength model, and report on what aspects of the multiscale model have been tested by these experiments, especially work hardening and dislocation mobility. [5] This is primarily a modeling talk, with some discussion of experimental validation. We consider experiments and simulations of deformation of polycrystalline Ta to study the role of Hall-Petch effects under extreme conditions. We also consider the orientation dependence flow stress in single crystal tantalum, and compare it to the MS model predictions. Finally, we discuss whether the MS model needs to be extended to include homogeneous nucleation. While the dynamic experiments generate integrated data, coupled with the detailed microphysics of the MS model simulations they are beginning to provide a compelling picture of the mechanisms of high-rate/high-pressure metal deformation.

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High-Temperature Discrete Dislocation Plasticity

Amine Benzerga

Texas A&M University, USA

A framework for solving problems of dislocation-mediated plasticity coupled with thermally-activated point-defect diffusion is presented. The dislocations are modeled as line singularities embedded in a linear elastic medium while a concentration field, as in continuum diffusion theory, represents the point defects. Plastic flow arises due to the collective motion of a large number of dislocations. Both conservative (glide) and nonconservative (diffusion-mediated climb) motions are accounted for. A variational principle is used to derive the coupled governing equations for point-defect diffusion and dislocation climb. Superposition is used at each instant to obtain the mechanical fields in terms of the infinite-medium solution for the discrete dislocations and an image field that enforces the boundary conditions while the point-defect concentration is obtained by solving the stress- dependent diffusion equations on the same finite-element grid. Aspects of the formulation are general but its implementation in a simple plane strain model enables the modeling of high-temperature phenomena such as creep, recovery and relaxation in crystalline materials. With emphasis laid on lattice vacancies, the creep response of planar single crystals in simple tension emerges as a natural outcome in the simulations. An adaptive time stepping scheme is used thus enabling to bridge the widely disparate time scales for dislocation glide and climb. A large number of boundary-value problem solutions are obtained which depict transitions from diffusional creep to power-law creep, in keeping with longstanding phenomenological theories of creep.

Tuning Ideal Tensile Strengths and Intrinsic Ductility of BCC Refractory Alloys

Liang Qi, Daryl Chrzan

Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA

Group 6 metal-based (Mo and W) refractory alloys are candidates as structural materials for many high-temperature applications. However, the lack of ductility at room temperature limits their applications. An important theoretical ductility criterion for these alloys is whether their nominally perfectly crystalline structures ideally fail by cleavage or shear deformation under tensile strain along [100] directions. Pure Mo and W fail by cleavage under [100] tension so that they are intrinsically brittle. Based on first-principles calculations and virtual crystal approximations (VCA), we found that decreasing electron numbers by alloying can make these alloys theoretically fail by shear instability and hence transform them into intrinsically ductile materials. This transition can be explained by a Jahn-Teller distortion, that lowers the total energy by splitting the degenerate energy levels of symmetry-related and partially-occupied orbitals. This discovery provides a guide for alloying processes aimed at increasing the intrinsic ductility of group 6 metal-based refractory alloys. This work is supported by EPRI.

DD Simulations of Temperature Effects on Tungsten Micro-pillar Compression with a Semi-phenomenological Dislocation Mobility Formulation

David Rivera, Giacomo Po, Tamer Crosby, Nasr M. Ghoniem

Department of Mechanical & Aerospace Engineering, University of California at Los Angeles (UCLA), 420
Westwood Plaza, Los Angeles, CA. 90095-1597, U.S.A.

The relation of the yield point and subsequent plastic behavior of BCC metals to the ductile to brittle transition temperature (DBTT) provides a unique opportunity to investigate the link between a clear macroscopically observed phenomenon (DBTT), and defect microstructure. The DBTT has been shown to be largely governed by dislocation mobility [1], or dislocation nucleation from crack tips [2]. This is attributed to the thermally activated kink-pair formation mechanisms governing dislocation motion in the low temperature regime. In this work, a dislocation mobility law is introduced and incorporated into a Dislocation Dynamics simulation package (MODEL), with the aim of elucidating the complex temperature governed interactions between defects which ultimately lead to either a brittle or plastic characterization of a BCC metal. The mobility law was obtained through careful analysis of experimental data found in literature, molecular dynamics simulations, and analytical theory for calculation of dislocation velocities in the high strain rate regime. The behavior of dislocations confined to a Tungsten micropillar is examined as a function of temperature and stress and compared to experimental results. The effects of variations in dislocation mobility are subsequently examined to reveal the pronounced impact temperature and stress combinations have on the plastic deformation of BCC metals.

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The subsonic/transonic transition of rectilinear edge dislocations: predictions from a field-based equation of motion

Yves-Patrick Pellegrini

CEA, DAM, DIF, F-91297 Arpajon, France

Atomistic simulations carried out during the last fifteen years have revealed the complexities of the behavior of accelerated edge dislocations. These include dramatic dynamic variations of core size, and depending on the type of loading applied, particular ways of leaping from subsonic velocities and "locking" onto asymptotically stable states of faster-than-shear-wave velocity [1]. So far, no fully satisfactory agreement between available models and such intricate results has been reported, even though useful theoretical information has been gathered.

Dislocation glide motion is that of a phase wave involving no transport of matter over more than atomic distances, accompanied by braking or acceleration wave emission. Because of this, dislocation inertia modelling at high velocities and accelerations escapes the classical Newtonian framework, which precludes using an equation of motion (EoM) with acceleration term proportional to some mass coefficient. A realistic EoM is all the more needed in view of recent advances towards truly dynamic discrete dislocation dynamics simulations [2}.

Recently, an approach based on a dynamic extension of the Peierls model delivered an EoM for the dislocation mean position that embodies most of the required wave physics [3]. However, the picture was not complete since an associated equation for the mean dislocation core evolution width was missing.

This talk summarizes our progress on this problem, introducing a new, closed, complex-valued EoM for the latter pair of collective variables [3]. Belonging to the class of retarded functional differential equations, our EoM includes retarded self-interactions, the aforementioned wave-emission effects, and provides fresh theoretical insights about dislocation inertia. Its main current limitation is that it cannot account for supersonic asymptotic steady states.

However, it allows one to investigate numerically the response of edge dislocations in fast-loading conditions of the single- and double-step types previously used in atomistic simulations [1]. In this context, we shall present a study of the subsonic-to-transonic transition of an edge dislocation, in good qualitative agreement with available simulations [1], including some non-trivial predictions for this transition that could be tested by atomistic methods.

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