

Editor's Choice

Accelerated molecular dynamics simulations for characterizing plastic deformation in crystalline materials with cracks



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ABSTRACT

Molecular Dynamics (MD) simulations are often used for comprehending evolving deformation mechanisms in materials at the atomic scale and also for assessing continuum-scale material properties. A major limitation of conventional MD simulations is that very small MD time-scale ($\sim fs$), restrict the achievable strain-rates to be much higher ($\sim 10^7$ or higher) than experimentally observed rates, needed for continuum scale modeling, e.g. using crystal plasticity finite element methods. A strain-boost hyperdynamics method based accelerated MD tool is adopted and developed to overcome these limitations. This method biases the atomic system to make it evolve at much faster time-scales and achieve strain-rates that are at least three order of magnitude smaller than the lowest strain-rate achievable in MD. The hyperdynamics algorithm is implemented in a parallel version of LAMMPS, and validated with conventional MD. It is then used to predict evolution of plastic state variables at lower strain-rates for a Nickel single crystal with an embedded atomistic crack. It is shown that at lower strain-rates, not only the evolution of plastic variables are different, but for some configurations there is a shift in the plastic deformation mechanism from twin dominated to dislocation dominated.

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1. Introduction

Deformation and failure behavior of metals inherently couple multiple spatial scales ranging from the atomic scale of defects and deformation mechanisms such as dislocations and twins to the continuum domains of grains and polycrystalline aggregates. Modeling the evolution of defects such as cracks and voids, their associated deformation mechanisms and interactions, often requires understanding and representation at the atomistic scales. Spatial and temporal coarse-graining of the atomistic behavior are subsequently needed to propose plasticity and damage constitutive relations at the continuum scale of single crystals. Molecular dynamics (MD) is one of the most effective simulation tools currently in use to investigate the behavior of many materials at atomistic scale. With increasing computational power, large scale atomistic simulations are routinely being conducted with several million or even billion atom systems, e.g. in [12,40] to study deformation and fracture in metallic systems. MD simulations have been used to study deformation mechanisms due to crack tip plasticity at finite temperatures in [37,38]. In [39] simulations have

been conducted at very low temperatures, thus eliminating any thermal activation and investigating only stress driven processes.

MD simulations used to study fatigue and failure are often faced with serious limitations in realizing experimental strain-rates. The typically achieved MD time-scales are in the *nano-*(ns) to *micro-seconds* (μs) range, corresponding to atomic vibrations with time-period in the order of *pico-seconds* (ps). Temporal resolutions required in the solution of the dynamical systems using incremental time-integration algorithms, limit the time-steps to be of the order of *femto-seconds* (fs). Even with today's powerful computing platforms, this limits the maximum physical time to the *micro-second* (μs) range. Correspondingly, in the study of deformation mechanisms in a deformable body, one is compelled to use very high strain-rates of $\sim 10^7$ or even higher to achieve strains of any physical significance. Thermal activation of stress-driven processes like nucleation of dislocations and microtwins make the mechanical behavior of materials temperature and strain-rate dependent. Very high strain-rates in conventional MD simulations can result in very different activation regimes compared to those in laboratory experiments. This leads to the activation of different temperature and strain-rate dependent deformation mechanisms like surface mediated dislocation nucleation [41]. High strain rate based MD simulations of fcc single crystal containing a crack in a certain orientation predicts a twin dominated deformation under

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mode-I loading, whereas room temperature experiments under similar loading do not show any twinning. This anomaly between experimental and simulation results has been attributed to the strain-rate effects in [36] where it has been shown that there is a transition from crack-tip twinning at short times to full dislocation formation at long times.

Various acceleration methods have been proposed in the literature to mitigate limitations of extremely small time-scales in MD simulations. These include the parallel replica dynamics or PRD method [30,35], the temperature accelerated dynamics or TAD method [27], and the hyperdynamics [33]. The hyperdynamics is one of the most effective time acceleration methods for predicting the temporal evolution of atomic systems. It has been used to study thermally activated nucleation processes like adatom diffusion on a substrate in [33] and also to investigate the stress driven thermally activated process like dislocation nucleation from sharp corners of a nanopillar in [8] and an atomic crack-tip in [3].

In the present work, the hyperdynamics-based accelerated MD method has been extended beyond the nucleation events to study deformation mechanisms in the plastic regime and quantify the evolution of plastic variables, which can be used in continuum based material models such as dislocation density-based crystal plasticity. The structure of the paper is as follows. A brief description of different time-scale acceleration methods are given in Section 2. In Section 3 different aspects of the hyperdynamics method are discussed with special focus on strain-boost hyperdynamics. Particular emphasis is on the construction of a boost potential with evolving parameters, as well as their implementation and validation. Finally in Section 5.2, a comparative study of the strain-rate effect is presented using high strain-rate conventional MD and low strain-rate hyperdynamics-based accelerated MD simulations.

2. Methods of time-scale accelerated molecular dynamics simulations

Various methods have been developed in the literature to achieve longer physical time-scales in MD simulations. A few of the important methods suitable for time acceleration of driven solid state systems are briefly discussed in this section.

2.1. The parallel replica dynamics (PRD)

The parallel replica dynamics or PRD method [35] is a simple yet accurate method that is based on the fact that most atomic processes are statistical in nature. It is based on the assumption that ensemble averaging over more micro-states is equivalent to exploring the system for longer time durations. This is achieved by temporal parallelization of the simulations over multiple processors, where individual processors run a replica of the sample independent of each other. This is in contrast with conventional parallelization, where the computational model is spatially distributed among multiple processors. The total number of micro-states explored in the PRD simulation process is sum from all the processors. Hence the accumulated simulation time (t_{phy}) is related to MD time of the individual i th replica (t_{MD}^i) as:

$$t_{phy} = \sum_{i=1}^{i=S} t_{MD}^i \approx S t_{MD} \quad (1)$$

where S is the total number of replicas and t_{MD} is the average time. It is obvious that the level of acceleration that can be achieved is approximately proportional to the number of processors (or replicas) used.

2.2. The temperature accelerated dynamics (TAD)

The temperature accelerated dynamics (TAD) [27] is a method of accelerating the time evolution of an atomic system, based on the observation that at finite temperatures an atomic system spends a substantial amount of time in the local potential well. Individual atoms vibrate with respect to their equilibrium position until an atom or a cluster of atoms acquire sufficient energy to overcome the local energy barrier and move to an adjacent potential well. The process continues until the system finds the global potential well. Material behavior is controlled by processes that are mainly stress driven and/or thermally activated. Thermally activated processes, which correspond to transition of a system from one local potential well to another, are inherently temperature dependent. Thus, the rate of this transition increases with temperature as the thermal energy available to overcome the energy barrier increases. To accelerate these transitions, simulations are performed at elevated temperatures but also by eliminating any spurious transition that does not occur at the original temperature. The speed-up or boost SU_{TAD} that is achieved by this method is expressed as:

$$SU_{TAD} = \exp \left[E_{min} \left(\frac{1}{K_b T_{low}} - \frac{1}{K_b T_{high}} \right) \right] \quad (2)$$

where E_{min} is the minimum energy barrier for state to state transition, T_{low} is the temperature at which the original MD simulation is intended, T_{high} is the elevated temperature at which the MD simulation is actually performed, and K_b is Boltzmann constant. A major challenge with this method is to come up with an appropriate criterion for filtering out the spurious transition, and extrapolating the state to state transition rate from an elevated temperature T_{high} to a lower one T_{low} .

2.3. Hyperdynamics (HD)

A very efficient way of accelerating the transition from one potential well to another for an atomic system had been proposed with the hyperdynamics or (HD) method in [34]. This method is based on lifting the basin of the potential-well or biasing the local potential landscape as shown in Fig. 1. A boost potential is added to the original system potential shown with the solid line to lift the potential well. The biased potential shown with the dashed line makes state to state transition more frequent i.e., at an accelerated pace. Time evolution of the biased system and the unbiased system can be related using the *Transition State Theory (TST)* [6,29,31]. From the TST and equilibrium statistical mechanics based ensemble-averaging it can be shown that time evolution of the

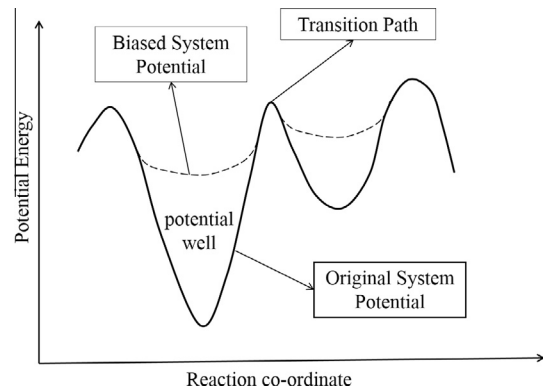


Fig. 1. Schematic illustration of the hyperdynamics method. The solid line corresponds to the original system potential, while the biased potential is shown with the dashed line.

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