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Molecular dynamics simulation of optimized shearing routes in single- and polycrystalline aluminum

Dirk Zahn *

Max-Planck Institut, für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany

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ABSTRACT

A recently developed approach to exploring cavitation and fracture processes from molecular dynamics simulations is transferred to shear deformation. The unprejudiced mechanistic analysis is demonstrated for two test cases, a single crystalline model of aluminum and a modified aluminum block. The modification is initially incorporated by removing an atomic layer from the single crystalline model. However, in the course of sampling the trajectory space of deformation routes, this deficient structure is optimized in favor of a polycrystal. For the latter model, our approach allows the investigation of shear deformation by dislocation slipping along the grain boundaries.

1. Introduction

The study of the atomistic mechanisms of deformation processes represents a fundamental contribution to the understanding of materials properties. In parallel to electron and atomic force microscopy, molecular simulation techniques promoted much of the in-depth knowledge available today. While atomistic detail and femto-second resolution is directly available to molecular dynamics simulations, the main limitation of this approach is related to accessing large model structures and long simulation time-scales.

Over several decades, a series of approaches were developed to tackle this time-length scale problem. A relatively new method for the study of energy barrier crossing events is represented by the transition path sampling (TPS) technique [1,2]. In the past years, a series of studies demonstrated the application to rare events such as nucleation, chemical bond reorganization and protein folding [3–6]. Moreover, the TPS scheme was recently transferred to cavity nucleation during fracture processes [7].

A key feature of the TPS approach is related to its unprejudiced convergence to favorable transition routes. Within an iterative sampling of trajectories, artificial starting pathways are optimized in favor of low energy. Typically, this evolution is most dramatic for the intermediate configurations required for the crossing of energy barriers. However, suitable implementation of the TPS scheme allows the optimization of all sketches of the trajectories, and may hence also be used to identify particularly favorable configurations in stable structures. An example for such an investigation is represented by our recent work on crystal formation from multinary melts which allowed insights into the local atomic arrangement of solid solutions and eutectic systems [8].

Following these developments [7,8], the aim of the present work is to further explore the perspectives of TPS molecular dynamics simulations in materials science. For this, the recently developed approach to exploring cavitation and fracture processes is transferred to shear deformation. Along this line, a particular focus is dedicated to the shearing of deficient structures and the unprejudiced optimization of the model systems to minimize the stress response to deformation.

2. Theory and simulation details

Analogous to our previous study on tensile deformation and fracture, the shear deformation processes investigated in the present work are mimicked by equilibrium molecular dynamics simulations. This is done by applying specific velocity profiles which are designed to induce spontaneous deformation to our model systems (Scheme 1). No external forces are applied, and our trajectories are obtained from constant energy molecular dynamics simulations. A physical interpretation of this model scenario may be given by deformation induced by finite temperature. To explore shear

* Tel.: +49 351 4646 4205; fax: +49 351 4646 3002.
E-mail address: zahn@cpfs.mpg.de

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deformation, we focus on a very particular temporary fluctuation giving rise to the desired process. Such momentum distributions are entropically disfavored and even in small model systems spontaneous deformation must be considered as extremely rare. Nevertheless, at sufficiently large total energy, such events are in principle possible and this condition is all what is needed at the initial stage of the TPS iterations.

Indeed, the artificially prepared pathways are only used as starting points for an iterative generation of further deformation routes. The TPS approach reflects a Monte-Carlo type sampling of the region of trajectory space corresponding to the process of interest [7]. As a consequence of this feature, the TPS iterations preferentially evolve to more and more realistic deformation routes. This convergence is further promoted by an additional favoring of low-energy pathways as described in Ref. [9]. By choosing obviously unfavorable starting pathways, the convergence of the sampling procedure may be nicely illustrated by the dramatic evolution of trajectories. As illustrated in Scheme 1, our initial pathways correspond to the collective motion of two halves in opposite direction. Such unlikely plastic deformation of the aluminum model is then optimized in favor of elastic deformation routes.

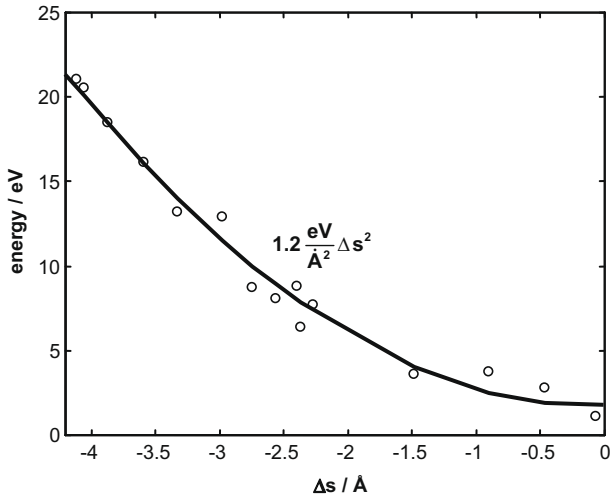

Fig. 1. Stress profile of the single crystalline model as a function of shearing. The shear modulus (at 0 K) is calculated as 19 GPa.

Each TPS iteration is implemented by randomly choosing an intermediate from the previous deformation trajectory. Conserving total energy and momentum, small momentum changes are applied (see Ref. [4] for details) and the new configuration is propagated in both directions of time. To ensure that these moves in trajectory space do not leave the desired regime of deformation pathways, only trajectories which fulfill a specific order parameter criterion are selected for further pathway production by repeating the above procedure. A suitable order parameter to describe shear deformation is represented by the dislocation of the upper and the lower faces of the model systems. For all studies discussed in the following, shear deformation by up to 5° was investigated.

Apart from this deformation criterion, no restrictions are imposed to the trajectory sampling. Typically, the optimization of pathways is most dramatic for the intermediate configurations of particularly high energy. However, this may affect all sketches of the trajectories, including the stable structures exhibiting no deformation at all. Unlike ideal single crystals, deficient structures comprise a large configurational manifold. In our simulations, this variety may be explored in terms of pathway optimization to low energy deformation routes. Similar to the evolution of the deformation mechanism, this also implies modifications of the structure to be deformed.

To illustrate both issues, we shall first study the deformation of a single crystalline block of aluminum. The underlying model was chosen as $10 \times 10 \times 20$ unit cells (8000 Al atoms, fcc structure with $a = 4.056$ Å) for which shearing is implemented along the [100] direction. To avoid additional effects arising from corners and edges, periodic boundary conditions are applied within the (001) plane. Shear deformation of this single crystalline model is then compared to a deficient structure which was generated by cutting a (001) layer of 140 atoms. Empirical interaction potentials [10] and a time step of 0.5 fs was used for the molecular dynamics simulations.

3. Results

The sampling of shear deformation pathways for both, the single crystalline model and the deficient structure, was initiated in the regime of plastic deformation routes as illustrated in Scheme 1. As expected for the single crystalline aluminum model, shearing by up to 5° is preferentially implemented by elastic deformation. After a few tens of TPS iterations, the block-wise shifting vanished

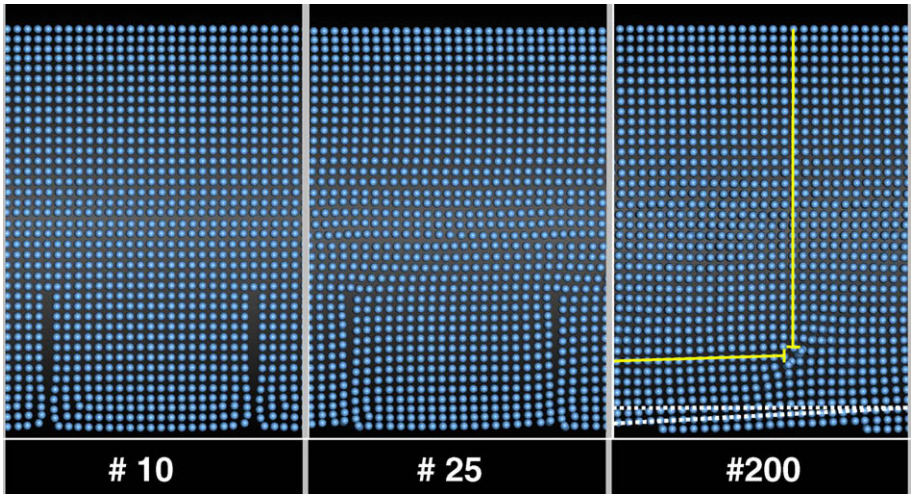

Fig. 2. Evolution of the deficient model system in the course of transition path sampling iterations. For each pathway, the shown snapshot is depicted at $\alpha = 0°$. After cutting an atomic layer, the optimized structure reflects a small angle grain boundary (tilt angle of about 3°) which is accompanied by two dislocations and the formation of steps in the formerly smooth surface.