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A New Simulation Method for Characterization of Mechanical Properties of Nanomaterials

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Abstract: A new simulation method has been developed and used to model mechanical properties of materials at many different length scales, from the nanoscale where an atomic description is appropriate, through a mesoscale where dislocation based descriptions may be useful to macroscopic length scales. In some materials, such as nanocrystalline metals, the range of length scales is compressed and a polycrystalline material may be simulated at the atomic scale. It is observed how the grain boundaries contribute actively to the deformation. At grain sizes below 5-10 nm deformation in the grain boundaries dominate over the traditional dislocation-based deformation mechanisms. This results in a reversal of the normal grain size dependence of the yield stress. It is shown that the material becomes softer when the grain size is reduced.

Key words: Simulation methods, mechanical properties, atomic scale, grain boundries, Iran

INTRODUCTION

Nanocrystalline metals are an attractive group of materials to model for many reasons. The materials are interesting from a technological point of view but also from a theoretical point of view since the small grain size results in a cut off of the typical length scales of the phenomena and structures that may appear during the deformation process. This simplifies, the deformation process and may possibly facilitate the development of theoretical models. Eventually, it may be possible to extend these models to the more complicated cases of coarse grained materials.

For the smallest grain sizes (below approximately 5-10 nm), it becomes possible to model the deformation process directly using atomic scale computer simulations (Clarke and Jonson, 1993).

The deformation processes may then be studied directly. Nanocrystalline metals are metals with grain sizes on the nanometer scale, typical grain diameters range from 5-50 nanometers.

These materials are of technological interest mainly because their strength and hardness often are far above what is seen in coarse-grained metals. This is generally believed to be caused by the grain boundaries acting as barriers to dislocation motion as the grain size is decreased, the number of grain boundaries increase and the dislocation motion becomes harder, leading to a harder material (D'Agostino and van Swygenhoven, 1996).

The simulation technique: We model the interactions between the atoms using a many-body potential known as the Effective Medium Theory (EMT) (Daw and Baskes, 1984). It is very important that the interactions are modeled using a realistic many-body potential such as EMT, the embedded atom method or the Finnis-Sinclair model (Gumbsch, 1995). Pair potentials such as Lennard Jones are still seen used for simulating metals due to the lower computational burden. Although, they give a good description of noble gas solid they are not adequate for modeling the bonding in metallic systems. One symptom of this is seen in the elastic constants, all pair potentials result in materials that satisfies the Cauchy relations between the elastic constants ($C_{12} = C_{44}$ for cubic crystals), a relation that is far from true in most metals. In the simulations, the samples are deformed by slowly increasing the system size along the z axis while minimizing the energy with respect to all atomic coordinates and with respect to the box dimensions in the x and y directions.

The minimization is done as a modified molecular dynamics simulation. After each time step, the dot product between the momentum and the force is calculated for each atom. Any atom where the dot product is negative gets its momentum zeroed as it is moving in a direction where the potential energy is increasing. This algorithm (Holt, 1970) is very efficient for this type of minimization. Before each time step, the system is stretched a little along the z direction. The two lateral dimensions are optimized by a Monte Carlo procedure

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every 20 time steps a change in the dimensions is proposed if the change results in a lower energy it is accepted, otherwise it is discarded. A few simulations were performed using the conjugate gradient algorithm for energy minimization (Jonsson and Andersen, 1988). The two algorithms were approximately equally efficient. During the simulation, the local stresses were calculated and stored for further analysis and the global values of the stress tensor were stored to generate stress-strain curves.

To facilitate the analysis of the simulations, the local order in the sample was analyzed. This was done using a method called Common neighbor analysis (Jonsson and Andersen, 1988). By investigating, the bonds between the neighboring atoms to the atom under investigation, the local crystal structure is determined. Atoms are then classified into three classes. Atoms in a local fcc order are considered ordinary bulk atoms; atoms in local hcp order are labeled as belonging to a stacking fault or the like and atoms in all other local orders are considered part of the grain boundaries or of dislocation cores.

RESULTS

Figure 1 shows the average stress-strain curves at each grain size. A clear grain size dependence is seen in the maximal flow stress. Figure 1 shows the maximal flow stress and the 0.2% offset yield stress in a standard Hall-Petch plot i.e., as a function of one over the square root of the grain size. A reverse Hall-Petch effect is clearly seen.

In Fig. 1, the stacking faults are present in several grains. They are created as partial dislocations (Shockley partials) move through the grains. They would be removed if a second partial dislocation followed in the same plane. This is, however rarely seen possibly because the grain size is comparable to the splitting width of the dislocation. Simulations of dislocation emission from a notch in a surface done by Jacobsen and Nielsen shown that the leading partial will move several splitting widths away from the notch, before the trailing partial is emitted. Possibly, a similar effect is seen here.

We have measured the amount of dislocation activity in the systems. The total dislocation activity is able to explain at most 2-3% plastic deformation i.e., less than half the observed plastic deformation. To identify the nature of the remaining deformation, we analyzed the relative motion of the individual atoms. The calculated shows the magnitude of the motion of the atoms obtained by subtracting the coordinates at two different strains (differing by 0.4%). The collective motion due to the imposed strain rate has been subtracted out. It is seen that the motion occurs mainly in the grain boundaries.

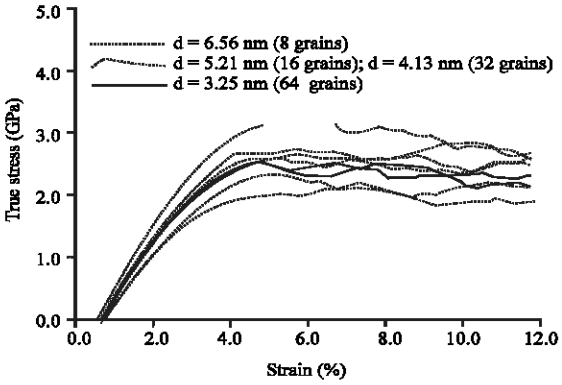

Fig. 1: Stacking fault in grain

An indication of the activity in the grain boundaries (Fig. 1) when the grain boundaries have become a little thicker during deformation.

CONCLUSION

It is demonstrated how atomic scale simulations can be used to obtain information about the deformation mechanisms in nanocrystalline metals. We find that at these grain sizes the dominating deformation mechanism is sliding in the grain boundaries through a large number of small events in the grain boundary. Each event only involves a few atoms. The result of this large number of small events is a flow in the grain boundaries, permitting the grains to slide past each other with only a minor amount of deformation inside the grains. The deformation mechanism results in a reverse Hall-Petch effect where the material becomes softer when the grain size is reduced. This is caused by an increase of fraction of the atoms that are in the grain boundaries as the grain size is reduced.

We have not yet been able to observe the cross-over between the range of grain sizes where this deformation mechanism dominates and grain sizes where a conventional deformation mechanism based on dislocation motion dominates. The hardness and yield stress of nanocrystalline metals is expected to reach its maximum in this cross-over region.

In order to simulate larger systems than the ones considered here, the atomic scale approach must be abandoned. We have provided an overview of simulation techniques at coarser scales and have indicated how they can be combined with atomic scale simulations to provide models of the mechanics of metals at multiple length scales. These techniques have not yet become main stream simulation tools but it is likely that many of them will gain more widespread usage in the near future.

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