SIMULATIONS OF NANOCRYSTALLINE METALS AT THE
ATOMIC SCALE. WHAT CAN WE DO? WHAT CAN WE TRUST?

J. Schiøtz

Center for Atomic-scale Materials Physics and
Department of Physics, Technical University of Denmark,
DK-2800 Lyngby, Denmark.

ABSTRACT

In recent years it has become possible to study the properties of nanocrystalline metals through
atomic-scale simulations of systems with realistic grain sizes. A brief overview of the main results
is given, such as the observation of a reverse Hall-Petch effect — a softening of the metal when
the grain size is reduced. The limitations of computer simulations are discussed, with a particular
focus on the factors that may influence the reliability of this kind of simulations.

1. INTRODUCTION

Molecular dynamics and other atomic-scale simulation techniques are providing much new under-
standing of various phenomena in materials science. A significant effort has been made to model
nanocrystalline metals using these techniques. The purpose and goals of such modelling is at least
twofold. On one hand, the materials themselves have technologically interesting properties, and a
better understanding of nanocrystalline materials is hoped to have direct technological relevance.
On the other hand, these materials provide a simplified model system useful for testing and devel-
oping theories about deformation in polycrystalline materials in general. The exceedingly small
grain size offers two advantages for theoretical studies. One is a suppression of large-scale struc-
tures in the grains, hopefully leading to a “simpler” material, the other is the possibility for direct
atomic-scale simulation.

Significant progress has been made in our understanding of the structure and mechanics of nano-
crystalline metals. For example, the grain boundaries are found to participate directly in the
deformation process of nanocrystalline metals, and at sufficiently small grain sizes they appear to
be carrying the majority of the deformation.
Less progress has been made on generalizing the results of atomic-scale simulations from nano-crystalline metals to more coarse grained metals. Direct extrapolation is likely to give a misleading picture, as new processes become active as the grain size is increased from the nanoscale. Many of the processes dominating the mechanics of coarse grained metals cannot occur within the tiny grains of a nanocrystalline metal.

This paper reviews the progress that has been made in the last few years using computer simulations to model nanocrystalline metals, and discusses the reliability of such simulations. For a more general review of nanocrystalline metals, see for example Morris (1998).

2. ATOMIC-SCALE SIMULATION TECHNIQUES

The main atomics-scale simulation techniques that have been applied to nanocrystalline metals are molecular dynamics and energy minimization techniques. In both cases, one starts with a description of the potential energy of the system expressed in the form of a “potential”, i.e. a function yielding the potential energy of an atom as a function of the positions of its neighbours. The potential must be carefully chosen in order to provide a realistic description of the bonding in the metal.

In molecular dynamics, one solves Newton’s second law numerically for the atoms in the system. Energy is thus preserved, and one obtains the positions (and velocities) of all the atoms as a function of time — the challenge is then to extract useful information from these data. Molecular dynamics can easily be modified to provide a well-defined temperature instead of a constant total energy.

Energy minimization techniques, sometimes known as “molecular statics” follow a similar idea. Instead of solving Newton’s second law the potential energy of the system is minimized with respect to all atomic coordinates. If this is done while changing an external parameter (for example the shape of the system) one obtains a “zero-temperature” simulation, describing how the system evolves in response to the external influence at a temperature of zero Kelvin.

The results of an atomic-scale computer simulation is typically many megabytes of atomic coordinates, velocities, and possibly other information such as atomic-scale stresses. Computerized analysis and visualisation tools are clearly necessary to make sense of such amounts of data. Sometimes the data is analyzed by calculating quantities similar to those obtained from experiments (for example radial distribution functions), and then use well-established experimental techniques to extract information about the structure of the simulated material. This is particularly useful if the calculated quantity is to be compared directly with experiments; but in many cases it goes against the “spirit” of atomic-scale simulations: that atomic-scale information is already present, and should be used directly.

Plotting the atomic structure directly, by drawing the atoms in a slice of the sample, is very useful, but must usually be augmented with further data analysis, such as selecting certain classes of atoms and/or coloring atoms according to stress, energy, displacement during the simulation, etc. A technique that has proven particularly useful in the context of nanocrystalline metals is the Common Neighbor Analysis (CNA), where the local crystalline structure around each atom is identified (Faken and Jönsson 1994; Honeycutt and Andersen 1987). This makes it relatively easy to identify grain boundaries, dislocation cores, stacking faults, etc.
3. MAIN RESULTS FROM ATOMIC-SCALE SIMULATIONS OF NANOCRYSTALLINE METALS

A number of papers reporting atomic-scale simulations of nanophase materials have been published in recent years (see for example Chen 1995; Derlet and Van Swygenhoven 2001; Heino and Ristolainen 2001; Keblinski, Phillpot, Wolf, and Gleiter 1997; Phillpot, Wolf, and Gleiter 1995a,b; Schiøtz, Di Tolla, and Jacobsen 1998a,b; Schiøtz, Vegge, Di Tolla, and Jacobsen 1998a,b; Van Swygenhoven and Caro 1997, 1998; Van Swygenhoven, Caro, and Farkas 1999; Van Swygenhoven, Spaczer, Caro, and Farkas 1999; Zhu and Averback 1996). In this paragraph some of the main results are reviewed.

3.1. Mechanical properties of nanocrystalline fcc metals. The mechanical properties of nanocrystalline copper, palladium and nickel have mainly been studied by Van Swygenhoven et al. and by Schiøtz et al. The three metals behave in a very similar way.

A series of simulations of plastic deformation of nanocrystalline copper has been published by Schiøtz et al. (1999a). The structure of one of the simulated systems is shown in Fig. 1. The structure shows evidence of some dislocation activity, such as the extrinsic stacking fault in Fig. 1b, which has been left behind by two partial dislocations (Shockley partials) moving through the grain. A detailed analysis of the dislocation activity during the deformation process indicates that the dislocations cannot be responsible for more than a quarter of the observed plastic deformation. The remainder of the plastic deformation is caused by a large number of apparently uncorrelated sliding events in the grain boundaries, see Schiøtz et al. (1999a) for details.

![Fig. 1: The initial (a) and final (b) configuration of a nanocrystalline copper system deformed 10% at 300 K. The system contains approximately 100 000 atoms arranged in 16 grains, giving an average grain size of 5.2 nm. Systems with smaller grain sizes were simulated with approximately the same number of atoms, while systems with larger grain sizes were simulated with ten times as many atoms to keep the number of grains sufficiently large. The arrow indicates where two partial dislocations have moved through a grain, leaving an extrinsic stacking fault behind. The majority of the plastic deformation has occurred in the grain boundaries.](image-url)
In coarse-grained metals, the plastic deformation is carried by dislocations, and the grain boundaries act as barriers to the dislocations. Reducing the grain size thus reduces the mobility of the dislocations, and leads to a harder metal. In nanocrystalline metals with sufficiently small grain sizes, the major part of the plastic deformation is carried by the grain boundaries — at least according to the computer simulations. It is, therefore, not surprising that decreasing the grain size leads to a softening of the metal, as the volume fraction of the grain boundaries increases. Based on the simulations, one can therefore predict that there should be an “optimal” grain size, where the hardness of a metal is maximal, see Fig. 3.

The simulations of Schiøtz et al. (1998a, 1999a) were performed at constant strain rate, typically $5 \times 10^8$ s$^{-1}$ (see section 5.2 for a discussion of these high strain rates). In the simulation one dimension of the simulation cell (the length) was controlled, while the two lateral dimensions were allowed to evolve in order to keep the lateral components of the stress near zero. The stress was calculated during the simulation to obtain the stress-strain curves. Van Swygenhoven et al. (1997) performed the simulations at constant stress, with periodic boundary conditions. 

Fig. 2: Stress-strain curves for nanocrystalline copper at 300K for varying grain sizes. The yield and flow stress is seen to decrease with decreasing grain size, this is summarized to the right. Adapted from Schiøtz et al. (1999a).

Fig. 3: Hardness of a metal as a function of the grain size. In the large-grain limit the hardness is given by the Hall-Petch relation $H = H_\infty + kd^{-1/2}$, in the other limit the hardness increases with grain size, indicating the existence of a maximum in hardness. On the figure the maximum has rather arbitrarily been placed at 10 nm. The position of the maximum is expected to vary with the material and probably also with strain rate, but is expected to be in the tens of nanometers. See also Nieh and Wadsworth (1991) and Yip (1998).
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1998, 1999) have performed simulations of plastic deformation of nanocrystalline nickel, where the applied stress has been the control parameter: a fixed stress was applied, and the dimensions of the simulation cell was allowed to evolve in time, yielding a “measured” strain rate. Strain rates in the order of $10^8$ s$^{-1}$ were seen; decreasing with increasing grain size. The observed grain size dependence of the strain rate is evidence of a reverse Hall-Petch effect.

### 3.2. Possible evidence for multiple deformation mechanisms

Assuming that the stress-strain relationship in nanocrystalline nickel is similar to the relationship in copper (see Fig. 2) one would expect a stress-dependent critical grain size for plastic deformation. If, for example, nanocrystalline copper were loaded with a tensile stress of 2 Gpa, one would expect that samples with a grain size below $\approx 6$ nm would flow, whereas samples with a larger grain size will exhibit some initial deformation which quickly stops. However, this is not quite what is observed by Van Swygenhoven et al. The strain rate is seen to decrease with increasing grain size, but at larger grain sizes it becomes approximately constant at a value of $\approx 10^7$ s$^{-1}$, independent of grain size. This is taken as evidence for a change in deformation mechanism (Van Swygenhoven et al. 1999). Apparently, a slower deformation mechanism is active in the regions of the stress-strain diagram in Fig. 2 which appear to be elastic. Evidence for such a mechanism was also reported by Schiøtz et al. (1999a): If the deformation is stopped while still in the “elastic” region, the stress is seen to relax exponentially with a relaxation time near 100 ps.

There is thus some evidence for two different, but closely related deformation mechanisms. The atomic-scale mechanisms appear to be very similar in the two cases, the main part of the deformation is carried by the grain boundaries (Schiøtz et al. 1999a, Van Swygenhoven et al. 1999). In the faster of the two mechanisms some dislocation activity is also seen in the grains. It is not clear if the slow mechanism can give rise to large deformations, or if it stops after a small strain has been created. It is possible that the slow deformation mechanism is not able to accommodate the small changes in grain shape, so the grains cannot efficiently slide past each others, whereas the limited dislocation activity seen in the faster mechanism allows such shape changes. This is, however, pure speculation as no computer simulations have been made where large deformations are obtained at a strain rate near $10^7$ s$^{-1}$ — molecular dynamics simulations of large systems is limited to times below a few nanoseconds. It is not unlikely that the two deformation mechanisms are essentially the same, but that similar small deformation events in the grain boundaries can be triggered both by thermal fluctuations and by the high stress. The two deformation mechanisms then corresponds to thermal activation or stress activation being dominant.

Unfortunately, there is no simulational evidence for the transition from the reverse to the normal Hall-Petch regime. It is expected that above a critical grain size, the majority of the deformation will be carried by dislocations moving inside the grains. However, little dislocation activity is seen even for the largest grain sizes. It is likely that an increase of the grain size from two to five times will be necessary to observe the normal Hall-Petch effect, requiring 10–100 times as many atoms, and correspondingly larger computers.

### 3.3. The structure of nanocrystalline metals

The structure of the grain boundaries in nanocrystalline metals has been a subject generating significant debate. It has been proposed that grain boundary structures of nanocrystalline metals are radically different from those in coarse grained metals. For example, a non-equilibrium low density structure has been proposed (Zhu, Birringer, Herr, and Gleiter 1987), but later experimental work is indicating that the grain boundaries are of high density, and not too different from those in coarse grained metals (Fitzsimmons, Eastman, Müller-Stach, and Wallner 1991; Stern, Siegel, Newville, Sanders, and Haskel 1995). Nevertheless, there
are significant uncertainties concerning the detailed grain boundary structure. A number of sim-
ulations have been addressing this question (Keblinski, Wolf, Phillpot, and Gleiter 1999; Phillpot et al. 1995a, b; Van Swygenhoven et al. 2000; Zhu and Averback 1996), reaching various conclu-
sions. Recently, Keblinski et al. (1999) found that the grain boundary structure is glassy without
much structure. They obtain this result by analysing the radial pair-distribution function of the
atoms in the grain boundaries. Van Swygenhoven et al. (2000) find that the grain boundaries con-
tain a lot of structure, with segments looking like coincidence site lattice boundaries, separated by
more disordered regions. They base their conclusions on direct visualisation of the grain boundary
structure, and argue that the less direct method of analysing the pair-distribution function is likely
to depend on the algorithm chosen to select the grain boundary atoms.

The question of the exact structure of the grain boundaries does not appear to have been settled
yet, but it should not be forgotten that the structure found in a simulation may depend on the
algorithm used to set up the grain structure in the first place (see section 5.4). If the structure
turns out to be independent of grain size, these results will also be of relevance for general grain
boundaries in coarse-grained polycrystalline metals.

4. FROM THE ATOMIC SCALE TO THE MACRO-SCALE.

Atomic-scale simulations cannot directly be applied to the deformation of everyday metals, as
the length scale of many important processes is far larger than anything that can be simulated
at the atomic scale. Simulating a volume of $1\mu m^3$ for a single second would require computers
that are $10^{12}$ times larger than anyone available today. Nevertheless, atomic-scale simulations can
contribute to the understanding of these materials as well.

Materials processes that are important in both nanocrystalline and coarse-grained metals can be
observed in simulations of the former. One example could be emission of dislocations from grain
boundaries and triple junctions, which is occasionally seen in the simulations. A detailed study of
those processes might reveal useful information about them, but no such work has to my knowl-
edge been published.

A more promising approach is to directly model fundamental processes that are known to be im-
portant, and where atomic-scale simulations may provide new information. One example is the
modelling of cross-slip of screw dislocations and annihilation of screw dislocation dipoles (Ras-
mussen, Jacobsen, Leffers, Pedersen, Srinivasan, and Jónsson 1997; Vegge, Rasmussen, Leffers,
Pedersen, and Jacobsen 2000, 2001). Further discussion of this and related work is beyond the
scope of this paper.

5. THE RELIABILITY OF ATOMIC-SCALE SIMULATIONS.

The main advantage of atomic-scale computer simulations is the unrestricted access to all atomic
coordinates. In principle, everything that happens can be determined with confidence from the
motion of all the atoms — although in reality the amount of information is so large that comput-
erized analysis and visualisation is necessary to extract information from the simulations.

The main disadvantage of computer simulations, atomic-scale or otherwise, is that one cannot be
sure how well they represent the reality they are supposed to reflect. This section discusses the

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main questions of reliability that must be considered in connection with atomic-scale simulations of nanocrystalline metals.

5.1. The precision and completeness of the underlying model. All computer simulations are based on an underlying set of assumptions and equations. Clearly, if the underlying model is incorrect, one cannot expect the computer simulation to give useful results. Many computer simulations rely on a large set of (explicit or implicit) assumptions about the processes going on in the system under investigation. For example, simulations in materials science often make assumption about the way plastic deformation occurs, how grains grow, etc; the weather forecast assumes a set of equations describing the hydrodynamics and thermodynamics of the atmosphere. In many cases the assumptions are well-founded and well-tested, but there is always the possibility that they do not apply in a given situation. For example, a simulation assuming that all plastic deformation occurs through the motion of dislocations would not have been able to find the reverse Hall-Petch effect mentioned previously.

One of the main virtues of molecular dynamics and related atomic-scale simulation methods is that the set of assumptions is very small. The simulation method does not assume anything about the processes occurring inside the material, as it is based on numerically integrating Newton’s second law while observing the motion of the atoms. The simulation will therefore not be biased by the user’s more or less well-founded assumptions about the processes occurring inside the material. For example, none of the simulations presented in section 3.1 assume that grain boundaries can slide or that dislocations can move (or even that dislocations exist, they appear “by themselves”). Even relatively exotic phenomena such as phonon-induced friction on the motion of dislocations are automatically included — whether they are important or not.

Unfortunately, this lack of bias in respect to which processes are important has a major drawback as well: the computational resources are not focussed on modelling the important processes. In the average molecular dynamics simulation a lot of effort is spent on resolving the thermal vibration of all the atoms. This leads to restrictions on the length and time scales that can be modelled, see section 5.2.

Although no assumptions are made concerning the important processes in the material under study, molecular dynamics is not completely independent of theoretical input. It depends critically on a reliable model for the interatomic interactions. The interactions are described by a potential: a function giving the potential energy of an atom as a function of the positions of the neighbouring atoms. The forces on the atoms are then found as the derivatives of the potential energy. The quality of the potential is obviously critical for the quality of the simulation.

The simplest choice for a potential is a pair potential, where the energy of an atom is given as the sum over the energy of the bonds to neighbouring atoms: \[ E_i = \sum_{j \neq i} E_{\text{bond}}(|r_j - r_i|). \] An example of such potentials is the Lennard-Jones potential, which gives a good description of the interactions between noble gas atoms, even in the solid phase, but is not suitable for most other condensed matter systems.

The interactions in a metal or a semiconductor cannot be approximated by a pair potential, more complicated functional forms are required. Most simulations of late transition metals use many-body potentials such as the Embedded Atom Method (EAM) (Daw and Baskes 1984) or the Effective Medium Theory (EMT) (Jacobsen, Nørskov, and Puska 1987; Jacobsen, Stoltze, and Nørskov 1996). They give a good description of a group of metals with face-centered cubic crystal struc-
ture, for example the EMT can describe the metals Ni, Cu, Pd, Ag, Pt and Au, and alloys between them.

In some situations no interatomic potential can describe the interactions with sufficient accuracy, and one has to use quantum mechanical calculations where the energy of the system being studied is found by solving Schrödinger’s equation for the electrons in the material. This is exceedingly time consuming, and limits the size of the simulation to around a hundred atoms. Fortunately, many materials properties do not depend in a sensitive way on the interatomic interactions, allowing one to use the less computationally expensive interatomic potentials. For example, the mechanical behaviour of nanocrystalline nickel, copper and palladium is experimentally very similar, and does therefore not depend critically on details in the interatomic interactions. One can therefore expect that a reasonable interatomic potential such as EAM or EMT will capture the essential physics. In situations where chemical effects seem to be important, such as various forms of chemical embrittlement, one has to be more careful and quantum mechanical methods may be necessary.

The amount of trust that can be placed in the description of the interatomic interactions should ultimately be determined by comparison with experiments, but in most cases must be based on the experience gained from similar simulations. It is the opinion of this author that in most simulations of nanocrystalline metals the potential gives a sufficiently accurate description of the interactions, and that the error introduced through the potential is probably smaller than errors introduced by other factors.

5.2. Limitations on the length and time scales. Since molecular dynamics works by numerically solving Newton’s second law for all the atoms, it captures all the motion of the atoms including the thermal vibrations. The time step used when integrating the equation of motion must therefore be very small. In typical simulations the time step is 5 femtoseconds or smaller. This limits the simulations to very short times, typically even a few nanoseconds of simulated time is computationally very expensive, at least for systems with many atoms.

One consequence of the short time-scale is that most diffusional processes are excluded from the simulation, as they occur on much longer time scales. In connection with nanocrystalline metals it means for example that diffusional creep cannot be observed in molecular dynamics simulations. Fortunately, experimental measurements of creep rates in nanocrystalline metals indicate that diffusional creep is not a large effect (Nieh and Wadsworth 1991; Nieman, Weertman, and Siegel 1991). Other thermally activated processes with activation energies near room temperature will also be suppressed by the short time scale. In many cases these processes can be identified for example by simulations at elevated temperatures, and then studied with more specialized simulation techniques.

As the time scale of the simulation is very short, very high strain rates are required to obtain an appreciable deformation during the simulation — strain rates around $10^8\text{ s}^{-1}$ are typically used, and one can be worried if this makes the results unreliable. The strain rate “gap” between simulations and experiment should not be ignored, but it is not an insurmountable obstacle. Although stress-strain curves of nanocrystalline metals are strain rate dependent both in experiments (Gray, Lowe, Cady, Valiev, and Aleksandrov 1997) and simulations (Fig. 4), the change in stresses is typically measured in percent (or tens of percent) when the strain rate is changed by several decades.

Since atomic-scale simulations are based on the individual atoms, the size of the system that
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Fig. 4: The effect of varying the strain rate in simulations of nanocrystalline copper with an average grain size of 5.2 nm. The same system was deformed at the same temperature (300 K) but at different strain rates, and the yield and flow stresses were extracted from the stress-strain curves. Both are seen to vary with the strain rate ($\dot{\varepsilon}$), strongest for $\dot{\varepsilon} > 10^9 \text{s}^{-1}$. Reproduced from Schiøtz et al. (1999a).

can be simulated is limited by the number of atoms that can be managed in the simulation. For realistic simulation, i.e. for simulations that cover more than a few picoseconds and use realistic interatomic potentials, the number of atoms is limited to a few tens of millions, even using the largest parallel computers. This severely limits the grain sizes of the polycrystalline metal under study.

Several methods have been proposed to overcome or circumvent these limitations. In the quasi-continuum method (Shenoy, Miller, Tadmor, Rodney, Phillips, and Ortiz 1999; Tadmor, Ortiz, and Phillips 1996) the number of degrees of freedom is reduced by using “representative” atoms to represent volumes of space where atomic resolution is not necessary. This allows for larger systems while maintaining atomic resolution in the relevant regions. Unfortunately, it is difficult to use quasi-continuum methods at finite temperatures (see for example Curtarolo and Ceder 2001).

A number of methods have also been proposed to deal with the limitations in time-scale. They all have in common that a correct description of the details of the atomic vibrations is sacrificed, while attempting to move the system between various states with the correct rates. Kinetic Monte Carlo (Voter 1986) and related methods require that all possible atomic-scale processes are known a priori, whereas hyperdynamics (Voter 1997a, b) and temperature-accelerated dynamics (Sørensen and Voter 2000) collect that information during the simulation.

5.3. Boundary conditions. As the number of atoms in a simulation is limited, one is effectively working with an exceedingly small sample. To limit the artifacts caused by the small sample one usually employs periodic boundary conditions, where the simulation cell is repeated infinitely in all directions. In this way no atoms are near free surfaces, and the system behaves as if it is deep inside the bulk of a material.

In some cases it is relevant to use free boundary conditions in some directions. For example, Derlet and Van Swygenhoven (2001) have simulated a nanocrystalline film by having free boundary
conditions in one direction, and periodic boundary conditions in the two other. They find that the surfaces cause an increase in the dislocation activity in the sample and a significant increase in the plastic deformation. The effects of the free surfaces appear to be localized in a layer of approximately the same thickness as the grain size. There do not appear to be qualitative changes caused by the free surfaces. In simulations of ultra-fast deformation of single crystals (Schiøtz, Leffers, and Singh 2001) film and bulk geometries are also seen to give qualitatively the same results, whereas wire geometry (with free boundary conditions in two directions and periodic boundary conditions in the third) give qualitatively very different results.

5.4. Initial configuration. Just as an atomic-scale simulation provides all details of the atomic motion during the simulation, it also requires all these details when starting. It is the responsibility of the user to provide a complete, atomic-scale description of the initial configuration of the material. This can be a major obstacle, as the full atomic configuration of real-world materials is rarely known, and can therefore be a major source of error in computer simulations. A bad initial configuration (a “bad sample”) can lead to distorted results — a problem simulations share with experiments!

The problem may sound more severe than it is, since in most cases details of the atomic configuration do not impact the macroscopic information that one wishes to gather from the simulation. For example, the positions of a few atoms may influence exactly when and where dislocations move through grains, but is unlikely to influence macroscopic quantities such as yield stress. Nevertheless, often simulations should be repeated with different initial configurations just as experiments are often repeated with different samples. In Fig. 2 the three lower stress-strain curves are the average over four different simulations with different, randomly generated grain structures.

Some ingenuity is normally required to generate realistic initial configurations. Several methods have been used to generate nanocrystalline samples. Phillpot et al. (1995a) generate a nanocrystalline sample by a computer simulation where a liquid is solidified in the presence of crystal nuclei, i.e. small spheres of atoms held fixed in a crystalline lattice. The system was then quenched a nanocrystalline metal was formed when the liquid crystallized around the seeds. The rapid solidification leads to a large number of stacking faults and other defects in the grains. Most other groups have generated the nanocrystalline samples using a Voronoi construction. A set of grain centers are chosen randomly, and the part of space closer to a given center than to any other center is filled with atoms in a randomly oriented crystalline lattice. The sample is then annealed briefly to remove unfavorable atomic configurations from the grain boundaries, see Schiøtz et al. (1999a) for details.

The samples generated by these methods are very “clean”, they do not contain impurity atoms or large defects like pores and voids. This is an advantageous simplification when the simulation is used to gain understanding of the deformation mechanism. But it is a disadvantage when comparing directly to experimental studies, where it is likely that impurities and defects are dominating the mechanical properties (see for example Agnew, Elliott, Youngdahl, Hemker, and Weertman 1998; Morris and Morris 1997; Sanders, Youngdahl, and Weertman 1997). Impurities can of course be introduced into computer simulations as well. As expected, porosity has a dramatic effect on the mechanical properties (Schiøtz et al. 1999a). Studies of impurities are limited by the lack of interatomic potentials giving a reasonable description of the embedding of a typical impurity atom (such as oxygen) in a metal. In a single study, silver has been introduced in the grain boundaries of copper with little effect (Schiøtz, Vegge, and Jacobsen 1999b).
5.5. Interpretation. Computer simulations rarely produce the desired new knowledge directly, considerable interpretation is usually required to extract the science from the simulation. There are, therefore, all the same possibilities for mis- and over-interpretations as is present in experimental work, although the full access to the atomic coordinates often makes the interpretation process easier and more reliable.

6. DISCUSSION AND CONCLUSIONS

Atomic-scale computer simulations can reveal important information about the deformation mechanism of nanocrystalline metals, information it would be difficult to obtain from other sources. Simulations have shown that the grain boundaries are participating directly in the deformation process, and if the grain size is sufficiently small the main deformation mechanism is grain boundary sliding, leading to a reverse Hall-Petch effect.

It can be difficult to evaluate the trustworthiness and reliability of computer simulations. There appears to be a large set of factors that can influence their reliability in a negative way. However, computer simulations are in that respect no different from most other techniques in materials science — most techniques, experimental or theoretical, have their own pitfalls. As a relative newcomer to the field, it is natural that atomic-scale computer simulations are greeted with some healthy scepticism. The atomic-scale focus of the technique places severe limitations on what can be done, but it also makes the approach relatively free from bias from its underlying models, allowing unexpected phenomena to appear in what is often called a “computer experiment”. If some care is taken when choosing the method and the subject under study, atomic-scale simulations can be a reliable source of information which would be difficult or impossible to obtain in other ways.

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