ELSEVIER

Materials Science and Engineering A 483–484 (2008) 33–39

MATERIALS SCIENCE & ENGINEERING A

www.elsevier.com/locate/msea

Footprints of plastic deformation in nanocrystalline metals

H. Van Swygenhoven

Materials Science and Simulation, ASQ/NUM, Paul Scherrer Institute, CH-5232 Villigen, Switzerland

Received 6 June 2006; received in revised form 19 October 2006; accepted 19 October 2006

Abstract

It now is possible to synthesize polycrystalline metals made up of grains that average less than 100 nm in size. Such nanocrystalline metals contain a significant volume fraction of interfacial regions separated by nearly-perfect crystals, a microstructure characterized by a significant high strength. This paper reports on a dislocation based deformation mechanism gained from insights obtained by atomistic computer simulations, followed by a discussion of some experimental observations.
© 2007 Elsevier B.V. All rights reserved.

Keywords: Nanocrystalline metal; Plasticity; MD simulation

1. Introduction

It is common knowledge that the mechanical behaviour of nanocrystalline (nc) metals is characterized by a significant increase in yield strength and a limited tensile elongation [1,2]. Fig. 1 compares the true stress–true strain behaviour up to failure of electrodeposited nanocrystalline Ni having a mean grain size of 30 nm with the behaviour of a coarse grained Ni (grain size >1 μm), the latter reaching total elongations of 20% and higher. The increase in strength with decreasing grain size is conventionally explained on the basis of dislocation pile-ups at grain boundaries, which directly leads to the Hall–Petch relationship relating the yield stress to the inverse square root of the average grain size [1,3,4]. Such an approach assumes implicitly the existence of dislocation sources and a dislocation multiplication mechanism providing the necessary dislocations for the pile-up. However, for small grain sizes the stress to bow out a dislocation might approach the theoretical shear strength [5] and the limited space offered by the nanocrystalline grains might strongly limit the operation of the usual multiplication mechanisms [6,7]. In other words, in order to understand the deformation behaviour of nanocrystalline metals in terms of dislocation activity, it is important to have a picture of possible dislocation propagation and multiplication mechanisms. In this keynote paper, we will first discuss the dislocation mechanisms suggested by large scale molecular dynamics of nanocrystalline f.c.c. metals with defect-free grain interiors. With this picture in mind, we will then report experiments performed on electrodeposited (ED) nc-Ni, finally discussing the level of current understanding and the open questions.

2. On the use of molecular dynamics

Massive parallel computing platforms offer the possibility to simulate multimillion atom samples using a molecular dynamics (MD) scheme and empirical potentials. It is now possible to simulate three-dimensional (3D) nanocrystalline structures with, for instance, 15 grains of 30 nm or 100 grains of 15 nm diameter, in other words, grain sizes of the same order as can be achieved experimentally [8]. The samples are usually built using a Voronoi procedure in which individual grains are geometrically constructed followed by a relaxation at room temperature [9]. Other procedures for the synthesis of 3D samples are used but they require more computing time [10–12]. When a special replica technique known as periodic boundary conditions is used, the sample can be considered as a small part of an infinite bulk nanocrystalline metal. In order to reduce the number of atoms in a simulation, samples with a two-dimensional (2D) columnar grain-boundary (GB) network have been constructed in which the periodic boundary conditions are applied on 10 atomic planes in the columnar direction [13,14]. In these samples the GBs are perpendicular to the tensile directions and contain only twist-free misorientations introducing additional simulation artifacts [15]. Fig. 2 shows a fully 3D computational sample representing nanocrystalline Ni with a mean grain size of

E-mail address: helena.vanswygenhoven@psi.ch.

0921-5093/$ – see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.msea.2006.10.204

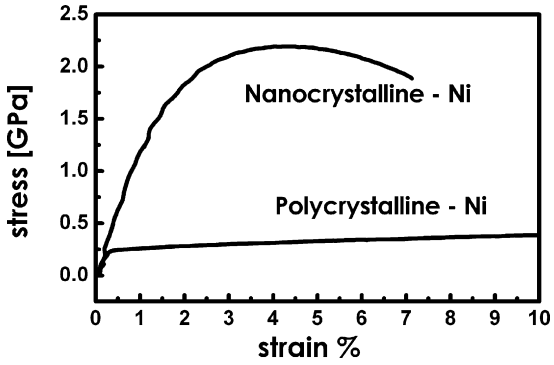

Fig. 1. True stress–true strain curves for ED-nc-Ni and coarse grained Ni. The coarse grained Ni reached a total elongation of 20%.

12 nm. The color code used is based on local crystallinity [16]: grey for atoms with an f.c.c. neighborhood, red for atoms with an hcp neighborhood, green for non-12 coordinated and blue for other-12 coordinated atoms.

Before interpreting results of MD simulations mechanism, it is important to summarize the inherent caveats of the MD technique, which have to be taken into account. A typical time step in MD has to be of the order of 1 fs, well below the vibrational period of an atom. Therefore, in order to reach a reasonable plastic deformation strain for an nc-sample with a sufficient number of grains in an acceptable computer time, one has to deform the sample with a minimum strain rate of 10^7 s^{-4}. This results in all kinds of possible high stress/short time artifacts [17] such as for instance the yield point observed in simulated stress-strain curves [18,19] in constant strain rate simulations and the usage of non-equilibrium strain rates for the determination of activation energies [20]. Moreover, it has also to be reminded that the short time step also restricts the amount of structural relaxation reached during computational sample synthesis, and therefore that all GBs in nc-samples have to be considered as non-equilibrium GB structures. It is therefore our view that the only meaningful information that can be extracted from simulations comes from a careful classification of the atomic processes taking place during deformation and not from the interpretation of simulated "macroscopic" stress–strain curves. Such an approach concentrates on revealing possible interactions between GB structure and deformation mechanisms in an nc structure.

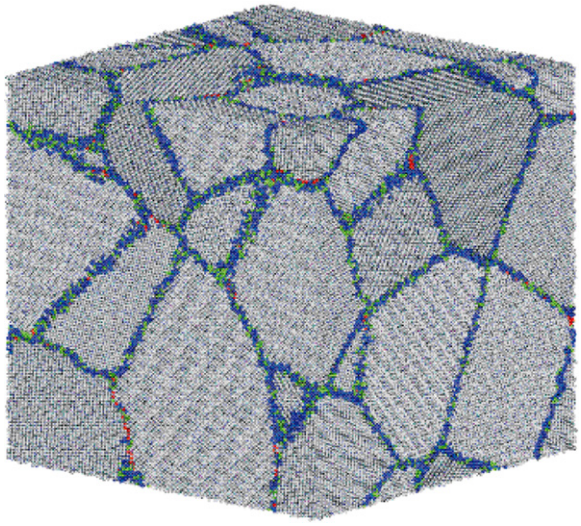

Fig. 2. Computer generated nanocrystalline Ni sample with a mean grain size of 12 nm synthesized using the Voronoi construction.

3. Deformation mechanism suggested by molecular dynamics

The dislocation activity revealed by MD is called "partial mediated" because single partial dislocations are emitted one at a time from the GBs. MD simulations using model potentials for Ni and Cu suggest that there is only one partial emitted that travels across the grain and leaves behind a stacking fault, whereas MD simulations for Al suggest a trailing partial follows, leading to the formation of a full dislocation or eventually a twin [21]. In an attempt to explain the suggestions from MD several models were proposed based on the absolute value of the stable stacking fault energy (SFE) and/or the equilibrium splitting distance [22–24]. Such an approach, while intuitively attractive, cannot explain all the simulation results since extended stacking faults are predicted for the material with the highest absolute value of the SFE. Moreover the splitting distance cannot be used as a nucleation criterion since it assumes the existence of both partials. Considering that there is no experimental evidence of the build up of a dense network of stacking faults after tensile deformation in nc-Ni and Cu and that in situ transmission electron microscopy (TEM) straining studies [25,26] reported "sudden contrast changes" which were interpreted to be the result of dislocation activity, one had to envisage possible simulation artifacts. The nature of this slip activity is now understood by considering the relative Peierls-type energy barriers for all possible partial dislocation-mediated processes represented through generalized planar fault (GPF) energy curves [21] for the empirical potential used. Given that the leading partial has already been nucleated, only full dislocations are observed in simulations for those materials having a ratio between the stable and unstable SFE close to unity. When twin structures are already present in the nc grains, a similar approach using the GPF curves explains how plasticity is affected by twin migration [27–29]. To explain how these simulations relate to experimental reality one has then to consider the short time aspect of the simulation. In the absence of impurities in the simulated GBs, local stress relief upon nucleation of the leading partial might delay nucleation of the trailing dislocation. For simulations using model potentials with a high ratio between unstable and stable stacking fault energy (such as Ni and Cu) the time to build up the stress concentration for nucleation of the trailing partial might not be reached within the simulation time. Taking into account the above arguments together with the lack in experimental evidence for a dense stacking fault network, one has to conclude that MD suggests a dislocation activity consisting of predominantly leading and trailing dislocations emitted and subsequently absorbed in the GBs, leaving behind no footprint. Fig. 3 shows an example of the typical dislocation mechanism suggested by MD. The grain segments in this picture

Download English Version:

https://daneshyari.com/en/article/1582237

Download Persian Version:

https://daneshyari.com/article/1582237

Daneshyari.com