letters to nature


Acknowledgements. We are grateful to G. J. Wasserburg, G. J. MacPherson and A. A. Ulyanov for providing samples of Allende and Efremovka CAIs for our study. We also thank E. J. Olsen of the Field Museum of Natural History for specimens of Murchison and Allende Trois which SH-7, BB-4, HAL and the seven hand-picked grains were extracted. We appreciate comments received from A. G. W. Cameron and E. Zinner. We acknowledge support from the Department of Space, Government of India (S.S. and J.N.G.) and from the National Aeronautics and Space Administration (A.M.D., L.G. and R.S.L.). J.N.G. also acknowledges hospitality provided by the Lunar and Planetary Institute, Houston, during the preparation of this manuscript.

Correspondence and requests for materials should be addressed to J. N. Goswami (email: goswami@pdl.ernet.in).

Softening of nanocrystalline metals at very small grain sizes

Jakob Schiøtz, Francesco D. Di Tolla & Karsten W. Jacobsen

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

Nanocrystalline solids, in which the grain size is in the nanometre range, often have technologically interesting properties such as increased hardness and ductility. Nanocrystalline metals can be produced in several ways, among the most common of which are high-pressure compaction of nanometre-sized clusters and high energy ball-milling. The result is a polycrystalline metal with a grain size of the order of a few nanometres. This grain size is determined by the size of the clusters used to prepare the material. The grains are typically randomly oriented. Atoms in local regions of the grains are located at grain boundaries and which are inside the grains. The grain boundaries act as barriers to the motion of dislocations, which results in a decrease in the flow stress of the material.

In this study, we used computer simulations to investigate the deformation of nanocrystalline metals. We used molecular dynamics simulations to study the deformation of nanocrystalline metals. We considered two different grain sizes, one of which was 3.3 to 6.6 nm and the other was 3.3 to 6.6 nm. We observed that the flow stress of the material decreased as the grain size decreased. This decrease in flow stress is due to the decrease in the number of grain boundaries per unit volume, which results in a decrease in the barrier to dislocation motion.

In conclusion, our results show that nanocrystalline metals can be used for applications where a high degree of ductility and high strength is required. These materials can be used in a wide range of applications, such as in the production of high-strength metals for aerospace applications, in the production of high-strength alloys for use in the automotive industry, and in the production of high-strength materials for use in the construction industry.

* Present address: SISSA, Via Beirut 2-4, I-34014 Trieste (TS), Italy.
required to allow for deformations of the grains, as they slide past each other. No dislocation motion is seen in Fig. 3, as none occurred at that time of the simulation. As the grain size is reduced a larger fraction of the atoms belongs to the grain boundaries, and grain-boundary sliding becomes easier. This leads to a softening of the material as the grain size is reduced (Fig. 2).

The observed deformation mode is in some ways similar to the manner in which grain boundaries carry most of the deformation in superplastic deformation17,18. This is consistent with recent simulations of flow speed in nanocrystalline metals25. However, in superplasticity the grain-boundary sliding is thermally activated, whereas here it occurs at zero temperature driven by the high stress.

In conventional metals an increase in hardness and yield strength with decreasing grain size is observed. This is called the Hall–Petch effect, and is generally considered to be caused by the grain boundaries, impeding the generation and/or motion of dislocations as the grains get smaller; this behaviour extends far into the nanocrystalline regime3,19. The grain sizes in the present simulations correspond to the smallest grain sizes that can be obtained experimentally. In that regime the Hall–Petch effect is often seen to cease or even to reverse, but the results depend strongly on the sample history and on the method used to vary the grain size. Many mechanisms have been proposed for this reverse Hall–Petch effect: increased porosity at small grain sizes5, suppression of dislocation pile-ups20, dislocation motion through multiple grains21, sliding in the grain boundaries22, and enhanced diffusional creep in the grain boundaries7. Direct measurements of the creep rates seem to rule out the last mechanism19,20, but otherwise no consensus has been reached. The present simulations indicate that the behaviour characteristic of a reverse Hall–Petch effect is possible even in the absence of porosity, and that it may be caused by sliding in the grain boundaries even in the absence of thermally activated processes. We cannot, however, see a cross-over from this 'reverse' behaviour to the normal Hall–Petch regime at larger grain sizes in our simulations, because they become too computationally expensive at these larger sizes. For the same reason, we cannot provide a direct comparison with the behaviour of the bulk metal.

A direct quantitative comparison between the simulations and the experimental results should be done with caution. The main difference between the simulated strain–stress curves and experimental curves is the level of the yield stress, which is approximately twice what is observed in experiments on low-porosity samples (400 MPa)13. This value is, however, obtained for a grain size of around 40 nm; extrapolation to 7-nm grains gives a yield strength around 800 MPa (ref. 23), assuming that the Hall–Petch behaviour persists to these grain sizes. Experimentally produced nanocrystalline samples typically contain voids and surface defects, reducing the strength of the material. Surface defects alone have been shown

Acknowledgements. We thank J. K. Nørskov, T. Lefers, O. B. Pedersen, A. E. Carlsson and J. F. Sethna for discussions. The Center for Atomic-scale Materials Physics is sponsored by the Danish National Research Foundation.

Correspondence and requests for materials should be addressed to J.S. (e-mail: schiotz@fysik.dtu.dk).