Mechanics and Mechanisms of Deformation

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For FY2003-2005 –

Graduate Students: 1

ABSTRACT AND BACKGROUND

The main objectives of this research effort are to develop (1) a fundamental understanding of the hierarchy of scales of events that occur during the deformation and failure processes of crystalline solids; and (2) an improved understanding of the underlying mechanisms for microstructural evolution in the solid state that are driven by the spatially and temporally inhomogeneous quantities spanning many different scales (e.g., primary recrystallization). The ultimate objective is the marriage of these two main objectives, so that deformation and solid-state phase transformations (e.g., dynamics of nucleation and growth of second phases) can be studied in a seamless manner with the accurate kinetic parameters of the evolution process. Current research efforts concentrate on developing 2D and 3D dislocation dynamics simulation algorithms to better elucidate the cooperative behavior of a very large number of dislocations, their reactions and self-organization and interactions with grain boundaries, point defects and second-phases at the meso-scale. We note that a number of researchers are currently pursuing 3D dislocation dynamics; however, relatively few researchers are examining the collective behavior of dislocations within the microstructures that are having interfaces and grain boundaries.

A portion of this effort is presented in the section, “Ductile Rare-Earth Intermetallics.”

Another portion of this effort is related to the understanding of homogenous and inhomogenous deformation behavior of metallic glasses and their composites and is presented in the Science of Amorphous and Aperiodic Materials section of this booklet.

TECHNICAL HIGHLIGHTS

- Calculated the role of grain size on strengthening of materials using dislocation dynamics.
- Progress has been made in the implementation of a level-set method for the purpose of studying phase evolution in the presence of mobile dislocations arising from the evolution of an internal stress field.
- Both interpolation and semi-analytical techniques were used to simulate the role of image forces on the dynamics of 3D dislocation segments near free surfaces. We observed changes in the attraction and repulsion rates of the dislocation from the free surface depending upon the character of the dislocation segments (screw, edge and mixed), the distance from the free surface and the length of the dislocation line. The simulation results also indicated that the magnitude of the applied stresses strongly influences the dislocation dynamics, and at moderate stress levels the contribution of the image forces becomes negligible for the dislocation motion.
- A constitutive model has been developed for void-containing and pressure-sensitive metallic glasses. With the constitutive model calibrated from the unit-cell analysis, the influence of a wide range of parameters: mechanical properties, volume faction and morphology of ductile reinforcements, on the ductility of metallic glass composites can be explored.

INTERACTIONS WITH OTHER PROJECTS AND PROGRAMS

A portion of this effort is integrated with the “Ductile Rare-Earth Intermetallics” effort. Efforts to develop simulation techniques for solid-state reactions (recrystallization, grain growth and evolution of second phases) by using deterministic and stochastic models are directly related to our work described in the Science of

Amorphous and Aperiodic Materials project, where we wish to understand the kinetics of phase evolution within the shear-bands.

A collaboration with D. Wolf at Argonne National Laboratory (ANL) was established in FY2001 on our efforts to understand and accurately simulate the evolution of grain growth and grain-boundary sliding during creep and superplastic deformation at the mesoscopic level. This effort is also now a part of the larger effort within the Computational Material Science Network (CMSN).

SELECTED PUBLICATIONS

S.B. Biner and J.R. Morris, "A Discrete Dislocation Simulation of Grain Boundary Strengthening," *Model. Sim. Mat. Sci. Eng.*, **10**, 617 (2002).

Y.Y. Ye, R. Biswas, J.R. Morris, A. Bastawros, and A. Chandra, "Molecular Dynamics Simulation of Nanoscale Machining of Copper," *Nanotechnology,* **14**, 396 (2003).

S.B. Biner and J.R. Morris, "The Effects of Grain Size and Dislocation Source Density on the Strengthening Behavior of Polycrystals," *Phil. Mag.,* **83**, 3677 (2003).

J.R. Morris, Y.Y. Ye, and M.H. Yoo, "An Ab Initio Calculation of the Structure and Energies of $\{10\underline{1}2\}$ Twin Boundaries in Zr, Ti and Mg," *Phil. Mag.,* **85**, 233 (2005).

S.B. Biner, "Ductility of Metallic Glasses and their Composites with Ductile Reinforcements: A Numerical Study," *Acta Mater*. (in press).

The Effects of Grain Size on the Strengthening Behavior of Polycrystals: The Dislocation Density Tensor Approach

Personnel: S.B. Biner (PI)

Scope:

> A dislocation pile-up model based on the dislocation density tensor approach was implemented into a 2D finite element code. This enabled study of strengthening behavior as a function of grain sizes ranging from 160μm down to 75nm and for up to 5% strains with extremely high computational efficiency. An inverse relationship between the grain size and 0.2% offset flow stress in the form of the Hall-Petch relationship is observed. The evolution of flow stress follows a narrow band when expressed as a function of dislocation density and hence suggests a scaling with the grain size.

Research Highlights:

We previously studied the grain-size strengthening behavior in polycrystalline solids by taking into account the collective behavior of a large number of discrete dislocations, on the order of 20,000, in a two dimensional setting [1,2]. The finite element method (FEM) implementation presented here is an extension of the earlier studies by Kroner [3] and Mura [4]. A continuous distribution of dislocations can be described by a dislocation density tensor such that:

$$\alpha_{ji} = \sum n \zeta_h b_i$$

where ζ is the unit vector tangent to the dislocation line, n is the number of dislocations per unit area with the same direction and $\boldsymbol{b}$ is the Burgers vector. The dislocations density tensor can be further related to the plastic distortion and the stress field associated with these plastic distortions (eigenstrains) can be obtained from the elasticity tensor. Determination of the total stress field due to dislocations and also due to remote boundary conditions then reduces to an internal stress problem in classical elasticity theory.

The FEM mesh used in our analyses to study the grain boundary strengthening behavior is shown in Fig.1a together with the simulated grain morphology and the location of the slip planes. During the simulations, both the grain morphology and the number of slip planes were kept constant. The analysis of grain sizes in the range of 160 μm to 75 nm was simply achieved by scaling the dimensions of the unit cell. The resulting displacement fields and distribution of shear stress for 160 μm grain size at 5% applied shear strain are shown in Figs. 1b and c, respectively. The inhomogeneity and the localization of deformation, and the resulting stress concentrations from the dislocation pile-ups at the grain boundaries can be clearly seen from these figures.

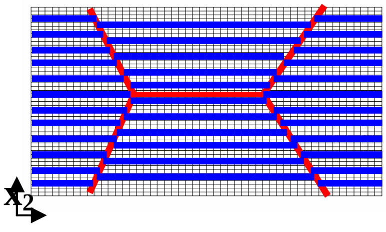

Fig. 1a

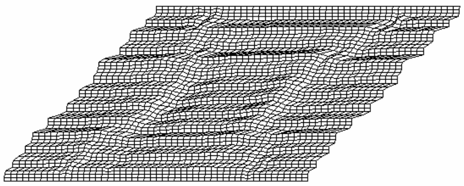

Fig. 1b

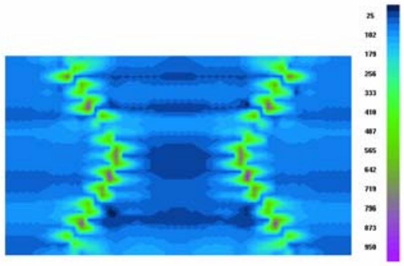

Fig.1c

The overall shear stress and shear strain response obtained from the simulations for all grain sizes are summarized in Fig. 2a. As can be seen from this figure, the initial response was elastic and yielding occurs at higher shear stress values with decreasing grain size. The work-hardening responses of each grain size with continuing deformation were also different. The correlation of the 0.2% offset flow stress (yield stress) with the reciprocal of the grain size *d*, for grain sizes spanning fours orders of magnitude, is plotted in Fig. 2b. The resulting slope of this log-log plot is shown to be 0.473, which is in close agreement with the standard $d^{-1/2}$ Hall-Petch correlation. In Fig.2c, the flow stress values are correlated with dislocation densities normalized with the grain size. As can be seen from this figure, the linear scaling with normalized dislocation densities with grain size is particularly good.

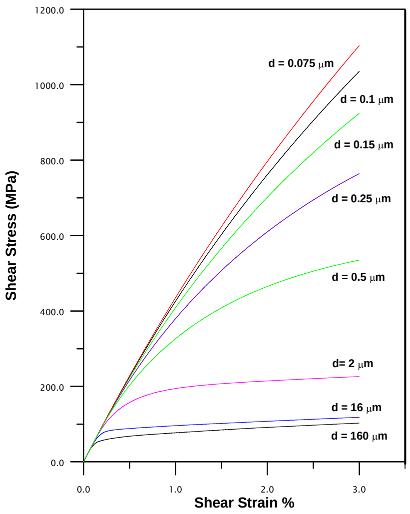

Fig.2a

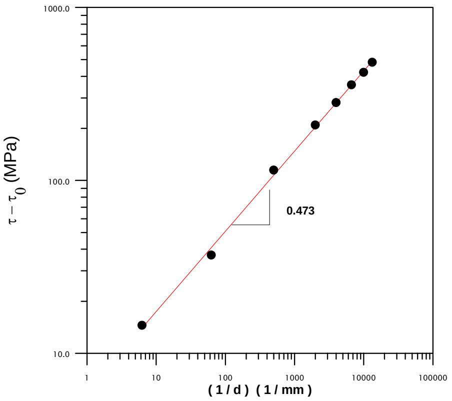

Fig.2b

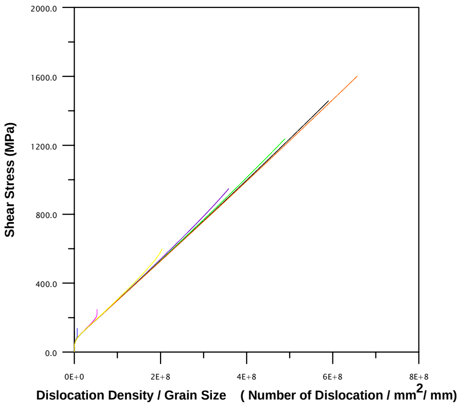

Fig.2c

Impact:

In the simulations presented, neither the dislocation sources nor the discrete dislocations and their reactions were implicitly modeled. The results support the many experimental studies of strengthening behavior, simply using the dislocation density while omitting the many details of the dislocation reactions that may take place during the course of deformation. The results are very comparable to our previous results based on discrete dislocation simulations [1,2], but require extremely less computation time. The linear scaling flow stress with normalized dislocation densities with grain size is particularly interesting, since it brings a length scale, for further development of the gradient plasticity theories.

Future Work:

The analysis including the multi-slip, cross-slip and sliding grain boundaries will be performed to elucidate the role of the grain sizes in the evolution of so called inverse Hall-Petch relationship.

[1] S.B. Biner and J.R. Morris, *J. Model. Simul. Mater. Sci. Eng.*, **10**, 617, 2002.
[2] S.B. Biner and J.R. Morris, *Philos. Mag.* **83**, 3677, 2003.
[3] E. Kroner, *J. Math. Phys.*,**42**, 27, 1963.
[4] T. Mura, *Micromechanics of Defects in Solids,"* Martinus Nijhoff Publishers, 1982.