

## ANISOTROPY IN POLYCRYSTALLINE TIN UNDER SIMPLE SHEAR

**A. Brydon<sup>a</sup> D. Sulsky<sup>a</sup> H. Schreyer<sup>b</sup> Y. Shen<sup>b</sup>**

<sup>a</sup>Department of Mathematics and Statistics  
University of New Mexico  
Albuquerque, NM 87131  
brydon@math.unm.edu, sulsky@math.unm.edu

<sup>b</sup>Department of Mechanical Engineering  
The University New Mexico  
Albuquerque, NM 87131  
schreyer@me.unm.edu, shenyl@me.unm.edu

As mechanical devices are made smaller, variations in material properties on the small scale play a significant role in determining the performance of the device. Direct simulations of small samples allow us to determine the influence of microstructure on macroscopic material properties. For example, we can study the effect of grain size, grain boundaries, or defects on the macroscopic behavior. It may also be possible to use simulations to develop new experimental techniques to test material properties of small samples.

Tin grains are tetragonal. In direct simulations of a few to thousands of grains in a polycrystalline sample, each grain is modeled with an anisotropic continuum, constitutive model. Each grain in the polycrystal is given a random orientation. For one such realization of grain orientations, effective moduli are computed, with particular attention paid to the shear modulus. Statistics are gathered for about 500 such realizations; both the average behavior of the tin samples and the variation in properties are examined.

Simulations on this scale are made possible by the use of a parallel implementation of the material-point method (MPM). The MPM uses two material descriptions, one is a Lagrangian description based on tracking a set of material points, and the other is an Eulerian description provided by a background computational grid. The purpose of combining these descriptions is to use each to best advantage while avoiding the disadvantages of each approach. We will provide an overview of MPM and its parallel implementation on distributed-memory architectures using MPI for communication.

Results will be reported for the elastic behavior of polycrystalline tin under simple shear. For tin samples composed of fewer than five hundred grains, the net behavior of the sample is shown to exhibit significant variations in effective shear modulus. The variations are also correlated with the grain size distributions. The resultant variations in effective shear modulus are compared with homogenization theory. While these models suggest a larger variation in properties, they are useful for providing bounds on the behavior at significantly less computational cost.

The full simulation of the polycrystal allows for examination of the internal stresses within the sample, and visualizations of this internal structure will be presented. Analysis of these stresses suggests that local values of stress can be significantly larger than suggested by the bulk properties. We also show that a measure of anisotropy based on the shear modulus correlates with the standard measure. In addition, preliminary analyses that include plasticity will be presented.