Crystal Models to Simulate Seeding of Rayleigh-Taylor Instabilities in Beryllium

We have implemented initial crystal-level modeling capabilities for beryllium in an existing framework. Capabilities include elastic, plastic, and thermal anisotropies related to the hexagonal crystal structure. These capabilities enable assessment of beryllium components under complex loading conditions such as those anticipated in NIF capsule implosions.

Project Goals

In this project, the primary sources of anisotropic response in beryllium are incorporated into existing crystal plasticity models available in the ALE3D finite-element program. We have also implemented enhancements for the incorporation of x-ray preheat data. We have tested capabilities, and built expertise in working with the models and interpreting results in light of interacting deformation mechanisms.

Relevance to LLNL Mission

Improved model descriptions for beryllium contribute to the capability to represent the general class of low-symmetry crystalline materials. A variety of programmatically important materials have low crystal symmetry. Capabilities for beryllium immediately benefit efforts for beryllium inertial confinement fusion capsules. For these beryllium capsules, x-ray preheat effects may have detrimental effects on surface roughness at the inner capsule surface and on perturbations within the bulk of the material. Anisotropic material response relates directly to the effects of interest. Perturbations that are exacerbated by material anisotropy play a role in the seeding of Rayleigh-Taylor instabilities, which are of concern in experimental physics studies of inertial confinement fusion.

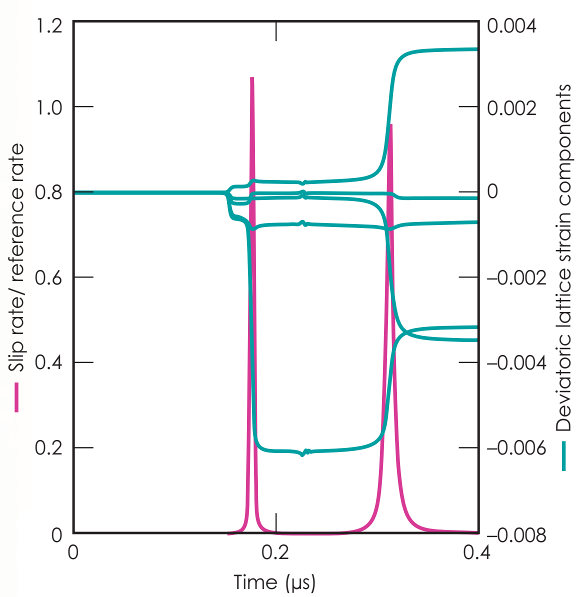

Figure 1. Time histories at a material location in a single crystal impact, showing plastic slip rate and lattice strain evolution. The elastic precursor is followed by two plastic waves. During the second plastic wave, there is a substantial shift in lattice strain, an effect related to plastic anisotropy.

Engineering Modeling and Simulation

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FY2005 Accomplishments and Results

ALE3D now includes a material model for beryllium that includes elastic, plastic, and thermal anisotropies. A capability has also been added for depositing x-ray preheat energy as a function of Lagrangian position. Model parameters have been calibrated using data from existing experimental work, and limited validation work has been performed using gas gun data.

The model reproduces the multiple plastic shocks observed experimentally at relatively low impact velocities, as shown in the 1-D single crystal impact results in Fig. 1. Complex material response is predicted for more general loading scenarios and microstructures. Results for a bicrystal are shown in Fig. 2, with considerable differences in break-out velocity for the two crystals.

Anisotropic thermal expansion alone can produce considerable nonuniform grain-level internal strains in a polycrystal, as shown in Fig. 3. These strains can lead to plastic deformation and the new capabilities allow for a first order assessment of this effect.

These new modeling capabilities have been tested in scenarios involving both spatially and temporally varying x-ray preheat and shocks induced by boundary loading. We have built expertise in interpreting material response under these combined loading conditions.

Related References

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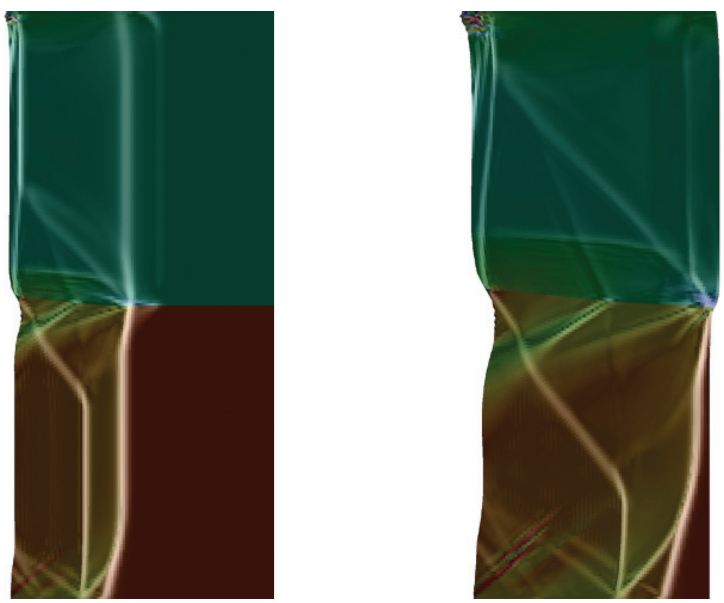

Figure 2. Results for a bicrystal at two time instances. Higher plastic strain rates are indicated by brightness; crystal lattice orientation is indicated by color. Loading is by an applied pressure on the left boundary; the right boundary is a free surface. Each of the two crystals initially has a uniform lattice orientation.

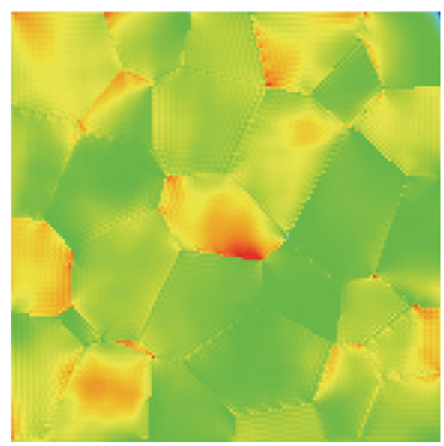

Figure 3. Lattice strain in a polycrystal due to temperature changes and anisotropic thermal expansion. Lattice strains are largest at grain boundaries where anisotropic expansion is accommodated.