Deformation of Low Symmetry and Multiphase Materials

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Materials composed of low symmetry crystals or of multiple solid phases exhibit heterogeneous deformation at the microstructural scale, often including deformation by mechanical twinning. Such heterogeneous deformation produces significant challenges in efforts to construct macroscale constitutive models, and necessitates careful attention in connecting to suitable experimental data. Heterogeneity at the microstructural scale also produces stress concentration that can lead to fracture or influence the onset and progress of phase transformations. We have developed an approach that explicitly incorporates effects of microstructure and deformation heterogeneity in a framework suited to analysis of engineering scale components.

Applications involving fully developed plastic flow are targeted. Basing polycrystal level models directly on experimentally measured microstructures, we build on recently developed technologies for effectively combining microscale plasticity simulations with macroscale models. This results in effective macroscale models for materials whose behavior is difficult to predict using conventional approaches. New capabilities capture the impact of microstructure, and thus material processing, on the performance of engineering scale components. For example, phenomena such as shear localization arise naturally.

Project Goals

Our overarching goal is to produce effective macroscale models through novel homogenization methods for a challenging class of materials. The immediate application space includes a wide set of engineering simulations, ranging from forming operations to dynamic loading scenarios. Figures 1 and 2 show example applications, with

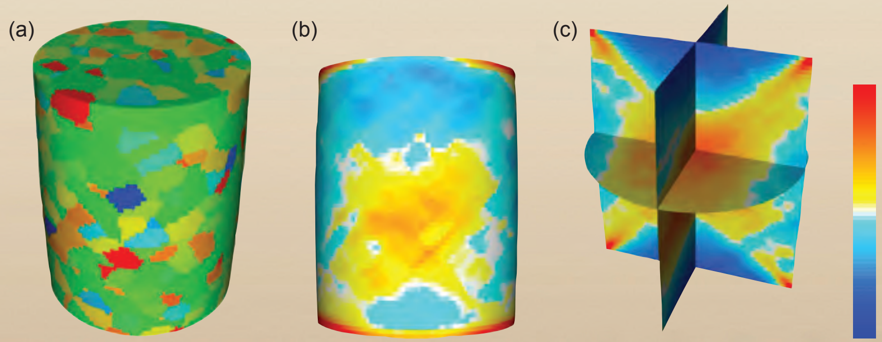


Figure 1. Results from a simulated Ti-6Al-4V compression test. (a) Long-range ordering of the microstructure associated with prior beta grain structure at elevated temperature. Strain localization patterns are shown in plots of the plastic strain rate (b) on the surface of the sample, and (c) on slices through the sample.

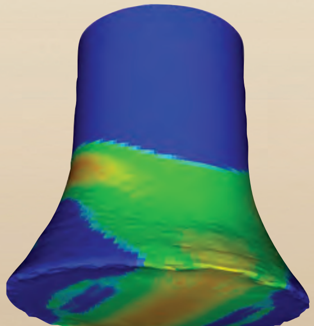


Figure 2. Simulation of a Taylor cylinder impact experiment showing plastic strain rate localization and the influence of plastic anisotropy, with coarse-scale and fine-scale state descriptors distributed as in Fig. 1.

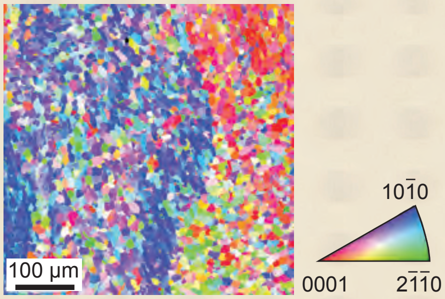


Figure 3. **Electron backscatter diffraction data, showing lattice orientation in the α phase of a Ti-6Al-4V sample. The plot is colored according to the crystal plane normal to the sample surface.**

computations informed by experimental data including measured microstructural information for the multiphase Ti-6%Al-4%V (Ti-6Al-4V) alloy (Fig. 3). Initial development focused on Ti-6Al-4V, given its widespread use and the availability of relevant experimental data. Software is developed in a component-oriented fashion, making use of tools that enhance parallel load balancing through task parallelism.

Relevance to LLNL Mission

The project aligns directly with the processing for performance and fracture components of the Engineering Simulation Roadmap and with Stockpile Stewardship Science needs identified in the more recently articulated LLNL Science and Technology Roadmap. Through the advancement of high-fidelity simulations and novel computational methods, the effort also aligns with high-performance computing and simulations aspects of LLNL's Science, Technology, and Engineering Pillars. We provide a more predictive modeling framework for a programmatically important class of materials, helping to close an identified capability gap.

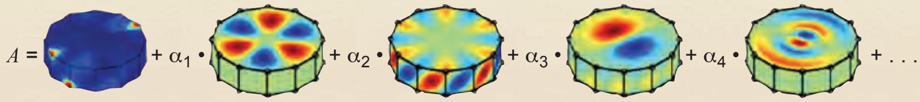
FY2009 Accomplishments and Results

In FY2009 we focused on increasing model fidelity by accounting for more detailed evolution of the state within the polycrystalline material. Within the efficient multiscale framework, we developed a method for evolving the probability density distribution of crystal lattice orientation based on finite elements over orientation space and discrete harmonics (Fig. 4). Evolution is governed by a partial differential equation over a non-Euclidean space, with nonlocal terms from twinning. The polycrystal level model can be either a simpler Taylor calculation or the Visco-Plastic Self-Consistent (VPSC) scheme developed at Los Alamos National Laboratory (LANL), which has been calibrated to a variety of materials of interest.

Deformation heterogeneity has been captured by discretizing individual grains in a polycrystal (Fig. 5), though this approach is computationally expensive and is not yet amenable to treating deformation by twinning. Twinning can be captured using a VPSC based approach, which also includes grain level deformation heterogeneity in the polycrystalline material.

Related References

1. Barton, N. R., J. V. Bernier, and J. K. Edmiston, "Bringing Together Computational and Experimental Capabilities at the Crystal Scale," invited presentation at *Shock Compression in Condensed Matter – 2009*.
2. Barton, N. R., J. Knap, A. Arsenlis, R. Becker, R. D. Horning, and D. R. Jefferson, "Embedded Polycrystal Plasticity and Adaptive Sampling," *International Journal of Plasticity*, **24**, pp. 242–266, 2008.
3. Bernier, J. V., N. R. Barton, and J. Knap, "Polycrystal Plasticity Based Predictions of Strain Localization in Metal Forming," *Journal of Engineering Materials and Technology*, **130**, 2008.
4. Barton, N. R., "Novel Algorithms in Computational Materials Science: Enabling Adaptive Sampling," *ASCR PI Meeting, U.S. DOE Office of Science HPCSW*, 2008.
5. Barton, N. R., J. V. Bernier, R. A. Lebensohn, and A. D. Rollett, "Chapter 11: Direct 3D Simulation of Plastic Flow from EBSD Data," in Electron Backscatter Diffraction in Materials Science, 2nd edition, Springer, 2009.



$$\frac{\partial A(\mathbf{r})}{\partial t} + \frac{1}{\nu(\mathbf{r})}\frac{\partial}{\partial \mathbf{r}} \cdot (A(\mathbf{r})\nu(\mathbf{r})\mathbf{u}(\mathbf{r})) = \phi(\mathbf{r})$$

Figure 4. **Schematic of the expansion of the probability distribution of crystal orientations in terms of discrete harmonics for the case of hexagonal crystal symmetry, such as in beryllium, magnesium, and zirconium.**

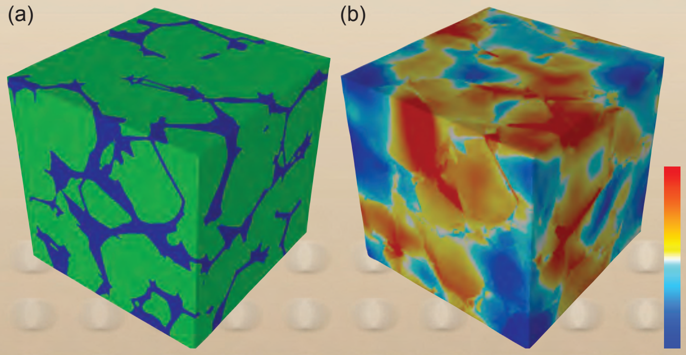


Figure 5. **Finite element calculation performed using ALE3D, showing (a) phase distribution and (b) strain localization with the average plastic strain rate seen in the white/gray areas.**