PRISM
NNSA Center for Prediction of Reliability, Integrity and Survivability of Microsystems

"Micromechanics of Polycrystals: Full-field Computations and Second-order Homogenization Approaches"

PURDUE UNIVERSITY Discovery Park

Friday January 27, 2012
3:00 pm, Birck 1001

Abstract: Models based on crystal plasticity are increasingly used in engineering applications. Three key elements of these methods are: 1) a proper consideration of the plastic deformation mechanisms at single crystal level; 2) a representative description of the polycrystal microstructure, and 3) an appropriate scheme to connect the microstates in the crystallites and the polycrystal response. The latter can be based on homogenization, which rely on a statistical description of the microstructure, or be full-field solutions, which requires a spatial description of the microstructure.

In the first part of this talk we will present a spectral formulation based on crystal plasticity and Fast Fourier Transforms (FFT) for the determination of micromechanical fields in plastically-deformed 3-D polycrystals. This formulation, pioneered by Suquet and coworkers [1] as a fast algorithm to compute the response of composites using as input a digital image of the microstructure, has been in turn adapted to deal with polycrystals deforming by dislocation glide [2,3].

Next, the FFT-based formulation will be used to assess the accuracy of different available nonlinear homogenization approaches for the prediction of the viscoplastic behavior of polycrystalline aggregates. We will show that Ponte Castañeda's second-order formulation [4], which explicitly uses information on average intragranular field fluctuations, implemented within the widely-used ViscoPlastic Self-Consistent (VPSC) code, yields the most accurate results [5].

[1] H. Moulinec, P. Suquet, Comput Meth Appl Mech Eng 157, 69 (1998).
[2] R.A. Lebensohn, Acta mater 49, 2723 (2001).
[3] R.A. Lebensohn, R. Brenner, O. Castelnau, A. Rollett., Acta mater. 56, 3914 (2008).
[4] P. Ponte Castañeda, J. Mech. Phys. Solids 50, 737 (2002).
[5] R.A. Lebensohn, C.N. Tomé, P. Ponte Castañeda, Phil. Mag. 87, 4287 (2007).

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Bio: Ricardo Lebensohn completed his Ph.D. in Physics in University of Rosario, Argentina, in 1993. After being a postdoc in the Polytechnic Institute of Grenoble, France, he returned to Argentina as professor and researcher of the National Research Council at the Physics Institute of Rosario. In 2003 he joined Los Alamos National Laboratory, where he is presently a senior scientist of the Materials Science and Technology Division, working in the area of modeling the structure/property relationship of crystalline materials. His contributions include the development of the ViscoPlastic Self-Consistent (VPSC) formulation and code. VPSC is a formulation based on non-linear homogenization for the prediction of texture evolution and texture-induced anisotropy of polycrystalline materials. The VPSC code is presently used for parameter identification, interpretation of experimental results and in multiscale calculations by numerous R&D groups worldwide. Dr. Lebensohn has also developed a spectral method for the prediction of full micromechanical fields in deformed polycrystals, using direct input from images of their microstructure. This efficient simulation tool is an ideal complement to emerging three-dimensional characterization techniques in experimental mechanics. Dr. Lebensohn recently received the Humboldt Research Award for "pioneering work in the field of multiscale modelling of plasticity of crystalline materials" and is a member of the editorial board of International Journal of Plasticity.