

# **Carnegie Mellon**

## **Materials Science and Engineering Seminar Series**

*Materials Research at Carnegie Mellon*

**Prof. Ricardo Lebensohn**

Los Alamos National Laboratory

*“A Formulation Based on Fast Fourier Transforms for the Prediction of Micromechanical Behavior and Microstructure Evolution of Plasticity Deformed 3D Polycrystals”*

**Friday, October 6, 2006**

**11:00 A.M. Seminar in Doherty Hall 1212**

*Refreshments precede seminar at 10:30 A.M. in 2325 Wean Hall*

We present a numerical formulation based on Fast Fourier Transforms to obtain the micromechanical fields in plastically deformed 3-D polycrystals. This formulation, developed in the last decade [1] as a fast algorithm to compute the elastic and elastoplastic response of composites using as input a digital image of their microstructures, has been in turn adapted to deal with 3-D polycrystals deforming by dislocation glide [2]. The FFT-based formulation provides an exact solution of the governing equations, has better performance than a Finite Element calculation for the same purpose and resolution, and can use voxelized microstructure data as direct input. To illustrate the capabilities of this model, we will show its predictions, together with comparisons with other models and experimental results on effective properties, local fields and average field fluctuations, subgrain structure formation, and global and local texture evolution in cubic and hexagonal materials.

[1] H. Moulinec, P. Suquet, "A numerical method for computing the overall response of nonlinear composites with complex microstructure", *Comput. Methods Appl. Mech. Eng.*, v. 157, p.69-94, 1998.

[2] R. Lebensohn, "N-site Modeling of a 3D Viscoplastic Polycrystal Using Fast Fourier Transform", *Acta mater.* v. 49, p. 2723-2737, 2001.

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Ricardo Lebensohn is a Researcher of the Materials Science and Technology (MST) Division at Los Alamos National Laboratory (LANL). Before joining LANL in 2003, he was an Associate Professor at the Physics Department of the National University of Rosario (UNR), Argentina, and a Researcher of the Argentina's National Research Council. He received his PhD degree in Physics from UNR in 1993, and did his postdoctoral training in Grenoble, France. In 1997, he was a Fulbright Scholar at UC Berkeley, and along his career he has been a Guest Scientist at: Technical University of Hamburg-Harburg (Germany), RISØ National Laboratory (Denmark), University of Paris-Nord and Ecole Polytechnique (France). He has been involved in research on Mechanics of Materials, especially in the area of modelling the mechanical behavior and microstructural evolution of complex heterogeneous materials, for over 15 years. He has published over 70 in peer-reviewed articles and given invited lectures at various International Conferences, Universities, Laboratories and industrial Research Centers in South America, United States and Europe.