998-65-163 **Luis A. Melara** (luism@cam.nist.gov), NIST, 100 Bureau Drive - Stop 8910, Gaithersburg, MD 20878-8910, and **Anthony J. Kearsley*** (ajk@cam.nist.gov), NIST, Room 375 - North, 820 Quince Orchard Road, Gaithersburg, MD 20899-0001. *Simulation of Twinned-Martensite as a PDE Optimization Problem.* Preliminary report.

Developing numerical methods for predicting microstructure in materials is an extremely large and important research area. Two examples of material microstructures are Austenite and Martensite. Austenite is a microscopic phase with simple crystallographic structure while Martensite is one with a more complex structure. One important task in materials science is the development of numerical procedures which accurately predict microstructures in Martensite near an Austenite-twinned-Martensite interface. In this talk we present two numerical approaches: one that involves the solution to an unconstrained optimization problem and a second that requires the solution to a constrained optimization problem. Numerical methods for solving both problems are presented together with a computationally affordable way of approximating the inequality constraint that appears in our second problem formulation. Preliminary results suggest that the minimizers of the constrained optimization problem display more desired characteristics. (Received February 24, 2004)