The Department of Mechanical Engineering/College of Engineering and Applied Sciences
Stony Brook University

Mechanical Engineering Seminar

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Lecture Title: Atomistic Molding of Martensitic Transformation in Shape Memory Alloys: Theoretical and Computational Techniques

Friday, April 25, 2008, 2:00 PM, Room 301 Engineering Building

Abstract

Some of the most interesting and technologically important solid-solid transformations are the first diffusionless (martensitic) transformations that occur in certain ordered multi-atomic crystals. These include the reconstructive martensitic transformations, where no group-subgroup symmetry relationship exists between the phases, found in steel and ionic compounds such as CsCl. Additionally, there are the reversible proper martensitic transformations, where group-subgroup relationships exist, that occur in shape memory alloys (SMAs) such as NiTi. SMAs are especially interesting, for engineering applications, due to their strong thermomechanical (multi-physics) coupling. The mechanism responsible for these stress-induced transformations is a change in stability of the crystal's lattice structure as the applied load is varied. The aim of this research is to understand the mechanisms that lead to the existence of these transformations. This is achieved by studying how simple atomic force models and exact crystalline geometry can give rise to truly complex properties of the bulk material. In this work, a continuum-level thermoelastic energy density for a perfect bi-atomic multilattice crystal is derived from an atomistic. Effective Interaction Potential (EIP) model. Cauchy-Born kinematics is used to ensure, by the introduction of internal atomic shifts, that each atom is in equilibrium with its neighbors. In order to identify any stress-induced martensitic transformations predicted by the EIP model the equilibrium equations are solved as a function of an applied load. Thus, a numerical branch-following technique is used to determine the quasi-static stress-strain behavior of the crystalline material. In addition, an asymptotic bifurcation analysis used to identify paths that emerge from all bifurcation points (simple and "multiple") that are encountered. The stability of each equilibrium configuration against all possible bounded perturbations is determined by calculating the phonon spectra of the crystal. One critical advantage of this approach is that the stability criterion includes perturbations of all wavelengths instead of only the long wave length information that is available from the stability investigation of homogenized continuum models. This allows one to capture the important "translation symmetry breaking" martensitic transformations often found in SMAs. The above described theory and methods will be reviewed and results will be presented that clearly demonstrate the EIP model's ability to simulate stress-induced transformations such as those found in common SMAs.

Biography

Ryan S. Elliott received his B.S. in Engineering Mechanics from Michigan State University. He received a M.S.E. in Aerospace Engineering, a M.S. in Mathematics, and a Ph.D. in Aerospace Engineering and Scientific Computing, all from The University of Michigan. In 2004 he was a Research Fellow at The University of Michigan, and in January 2005 he joined the faculty of the Aerospace Engineering and Mechanics Department at The University of Minnesota. Elliott's research interests are in the areas of active materials and shape memory alloys. Specifically, he studies the detailed atomic scale behavior of martensitic transformations using bifurcation and stability techniques. Dr. Elliott has received numerous awards, including: the Tau Beta Pi Matthews Fellowship (1998), the U.S. D.O.E. Computational Science Graduate Fellowship (2000), the Ivor K. McIvor Award in Applied Mechanics, the Frederick A. Howes Scholar in Computational Science award (2005), and a National Science Foundation CAREER grant (2007). Elliott's research has been presented at numerous national and international conferences.

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