Equilibrium Path-following, Bifurcation, and Stability Techniques for Studying Temperature-Induced and Stress-Induced Martensitic Transformations in Crystalline Shape Memory Alloys

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Some of the most interesting and technologically important solid-solid transformations are the first-order 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 such as NiTi. Shape memory alloys are especially interesting, for engineering applications, due to their strong thermomechanical (multi-physics) coupling. The mechanism responsible for these temperature- and stress-induced transformations is a change in stability of the crystal's lattice structure as the temperature is varied.

My research aims to understand the mechanisms that lead to 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 a set of temperature-dependent atomic pair-potentials. The Cauchy-Born kinematic assumption is used to ensure, by the introduction of internal atomic shifts, that each atom is in equilibrium with its neighbors. First, temperature-induced transformations are investigated. Path-following techniques are used to determine stress-free equilibrium crystal configurations as a function of temperature. An asymptotic bifurcation analysis identifies 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. The advantage of this approach is that the stability criterion includes perturbations of all wavelengths instead of only the long wavelength information that is available from the stability investigation of homogenized continuum models. Secondly, stress-induced transformations at constant temperature are studied. The response of the model to uniaxial loading is determined using the same path-following, bifurcation, and stability techniques.

In this talk, I will review the above described methods and present results. These include the prediction of a hysteretic two-step temperature-induced proper martensitic transformation from a high-temperature B2 cubic (austenite) phase, to an intermediate (alpha)IrV orthorhombic phase, to a final B19 orthorhombic (martensite) phase. Stress-induced transformation, at high temperature, between the B2 cubic and (alpha)IrV structures is also predicted. The existence of both temperature- and stress-induced transformations indicates the possibility for shape memory behavior. Finally, the predicted transformation parameters show good correspondence with experimental values for the shape memory alloys CuAlNi and AuCd.