Stress-induced martensitic transformations in perfect bi-atomic crystals

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Solid-to-solid martensitic phase transformations are technologically important phenomena that result in unique macroscopic material properties such as the shape memory effect, ferromagnetism, and ferroelectric behavior. In shape memory alloys, such as CuAlNi and NiTi, the martensitic transformation can result from a change in temperature or the application of stress. In fact, *both* temperature-induced and stress-induced transformations are essential for the existence of shape memory behavior.

In previous work we proposed an atomic model for bi-atomic alloys based on a set of temperature-dependent atomic pair-potentials. An innovative bifurcation and stability technique was used to numerically investigate the model and a proper temperature-induced martensitic transformation was discovered. The transformation involves a $B2$ cubic austenite phase that deforms into a $B19$ orthorhombic martensite phase via a uniform deformation of the crystal lattice as well as internal atomic shifts. These results were compared to experimental data for real shape memory alloys that undergo the same $B2$ to $B19$ transformation (CuAlNi and AuCd) and surprisingly good quantitative agreement was found.

The current investigation aims to identify the existence of a stress-induced martensitic phase transformation associated with the same set of atomic potentials. The previous bifurcation method is used to map the set of connected equilibrium crystal structures, both stable and unstable, for a $B2$ cubic crystal subject to an applied $< 110 >$ uniaxial stress. Special attention is paid to the choice of internal atomic shift degrees of freedom to ensure that all equilibrium paths of interest are identified. It is found that hundreds of equilibrium paths exist corresponding to crystal structures of orthorhombic, monoclinic, and triclinic symmetry. Nearly all of these equilibrium structures are unstable and, therefore, unobservable in nature, but there exists a small subset of paths that correspond to stable phases of the material. These low symmetry phases indicate the existence of a stress-induced proper martensitic transformation for the material.

This talk will first provide an overview of the current atomic model and review previous investigations of the stress-free temperature-induced transformation behavior. Then a description of the numerical results for stress-induced transformations will be presented with a discussion of the transformation's characteristics, including transformation strains and hysteresis.