

The Southwest Mechanics Lecture Series

at

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THERMALLY INDUCED MARTENSITIC TRANSFORMATIONS IN ATOMIC LATTICES

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A well-known feature of some metallic alloys, such as NiTi, is their thermally induced, stress-dependent shape memory behavior. These alloys' remarkable properties are due to one or more martensitic transformations near room temperature, in which the crystalline configuration changes from a higher symmetry austenite (cubic lattice), to a lower symmetry martensite (rhombohedral, orthorhombic, tetragonal or monoclinic lattice) with decreasing temperature.

In contrast to existing phenomenological approaches, the present work consists of obtaining the continuum energy density function $W(\mathbf{F}, \theta)$ (where \mathbf{F} is the lattice's uniform deformation gradient and θ its temperature) of a perfect periodic bi-atomic lattice from temperature-dependent atomic potential functions. Of interest in this work are the equilibrium solutions and their stability for stress-free crystals as functions of temperature. Although the full problem is solved numerically, an asymptotic theory is necessary to guide the numerical solution near the inevitable multiple bifurcation points. For a particular choice of the atomic potentials, we find that the stability of the austenitic phase changes at a critical temperature θ_c . Depending on the multiplicity n of the eigenvalue at the critical temperature, one can have three (for $n=2$) or seven (for $n=3$) bifurcated equilibrium branches. In the first case ($n=2$) the three branches correspond to tetragonal phases while in the second case ($n=3$) three branches corresponding to orthorhombic and four branches corresponding to rhombohedral phases. Similar analyses give monoclinic bifurcated branches emerging as secondary bifurcations from the above described rhombohedral or orthorhombic primary branches. These analytical asymptotic solutions near the multiple bifurcation points guide (and confirm when possible) the complicated numerical results obtained in the case of a pair potential example for a bi-atomic lattice.