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Stability of crystalline solids—II: Application to temperature-induced martensitic phase transformations in a bi-atomic crystal

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Abstract

This paper applies the stability theory of crystalline solids presented in the companion paper (Part I) to the study of martensitic transformations found in shape memory alloys (SMA's). The focus here is on temperature-induced martensitic transformations of bi-atomic crystals under stress-free loading conditions. A set of temperature-dependent atomic potentials and a multilattice description are employed to derive the energy density of a prototypical SMA ($B2$ cubic austenite crystal). The bifurcation and stability behavior are then investigated with respect to two stability criteria (Cauchy–Born (CB) and phonon). Using a 4-lattice description five different equilibrium crystal structures are predicted: $B2$ cubic, $L1_0$ tetragonal, $B19$ orthorhombic, $Cmmm$ orthorhombic, and $B19'$ monoclinic. For our chosen model only the $B2$ and $B19$ equilibrium paths have stable segments which satisfy both the CB- and phonon-stability criteria. These stable segments overlap in temperature indicating the possibility of a hysteretic temperature-induced proper martensitic transformation. The $B2$ and $B19$ crystal structures are common in SMA's and therefore the simulated jump in the deformation gradient at a temperature for which both crystals are stable is compared to experimental values for NiTi, AuCd, and CuAlNi. Good agreement is found for the two SMA's which have cubic to orthorhombic transformations (AuCd and CuAlNi).

Keywords: Phase transformation; Finite strain; Stability and bifurcation; Asymptotic analysis

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1. Introduction

The stability theory of crystalline solids using multilattice kinematics has been discussed in the companion paper Elliott et al. (2004b) (henceforth referred to as Part I), where three different stability criteria were presented and compared. Here an application of this theory to martensitic transformations that occur in shape memory alloys (SMA's) is considered. As a first step, the focus is on temperature-induced martensitic transformations under stress-free loading conditions.

Martensitic transformations (MT's) according to Cohen et al. (1979) are diffusionless lattice-distortive phase transformations of the crystal. That is, during a martensitic transformation the atoms of a highly ordered crystal rearrange in a coordinated manner leading to a new crystalline phase. These transformations are often temperature-induced and may occur over a wide range of temperatures. The high temperature phase is called *austenite* and the low temperature phase is called *martensite*. In the materials science literature MT's are often further subdivided into those which are reversible (or thermo-elastic) as for SMA's and those which are irreversible as for martensitic steels.

Here a somewhat different view is adopted, as proposed in Elliott et al. (2002b), where MT's are partitioned into two categories called *proper MT's* and *reconstructive MT's*. Proper MT's are identified by the austenite and martensite crystals having a group-subgroup symmetry relationship. This has been shown to be a necessary feature for a material to exhibit a shape memory effect (see Bhattacharya, 2003), since it guarantees that austenite is a unique configuration to which martensite can revert. Additionally, if high symmetry austenite and low symmetry martensite configurations are connected by an infinitesimal deformation, the so-called Ericksen–Pitteri neighborhood (Ericksen, 1978; Pitteri, 1984; Bhattacharya, 2003), the phase transformation is likely to be reversible upon cooling or heating in some neighborhood of the transformation temperature. In a reconstructive MT, by contrast, no group–subgroup relationship exists between the crystal configurations. Although not considered diffusional, the transformation involves significant atomic motions with breaking of nearest-neighbor bonds and then bond reformation (Tolédano and Dmitriev, 1996), often resulting in significant dilatational changes of the crystal. Reconstructive MT's exist in many materials, including steel, many of the pure elements, and ionic compounds such as CsCl, NaCl, and other alkali-halides. Reconstructive MT's were successfully simulated in Elliott et al. (2002b), where a set of temperature-dependent Morse pair-potentials were used to investigate the uniform (affine) deformation of a bi-atomic $B2$ crystal structure, and an MT between the cubic $B2$ and cubic $B1$ crystal structures was simulated.

Martensitic transformations have been a subject of active study for many decades. In 1937 *L. D. Landau* developed a phenomenological theory of phase transitions including MT's (see, for example, Dove, 1993). This theory has successfully modeled the properties of known phase transitions (see, for example, Bruce and Cowley, 1981; Dove, 1993). In Landau theory the "free energy" of the crystal is expanded as a polynomial function with temperature-dependent coefficients of an "order parameter" that measures the extent of transformation. The form of the free energy is constrained to satisfy certain symmetry relations for the crystal of interest. Phase transformation is assumed to occur at the temperature where the free energy of the austenite phase becomes equal to the free energy of the martensite phase.