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Bifurcation Techniques for Structural Phase Transitions RYAN S. ELLIOTT, University of Minnesota, JOHN A. SHAW, NICOLAS TRIANTAFYLLIDIS, University of Michigan — A new technique for studying structural phase transitions in crystals has been developed which uses bifurcation theory to investigate a material's free energy landscape. In this method a material's behavior is numerically interrogated by beginning with its high temperature structure and mapping out the equilibrium branch corresponding to the distortions of the crystal structure that occur due to changes in parameters such as temperature or stress. The investigation of this equilibrium branch is continued into unstable regions of the material's free energy landscape, i.e., regions which are physically unobservable. In these unstable regions the equilibrium branch bifurcates, or splits, and leads to other stable regions corresponding to different crystal structure branches (phases), thus revealing the links and interactions between the various phases of the material. Often, unexpected stable phases are identified in this way. It is common to encounter non-generic bifurcation points, where a single equilibrium branch splits into many (instead of two) new equilibrium branches. In these complex situations, the current bifurcation method is guaranteed to systematically identify all of the new branches. To illustrate the method, an atomistic model for shape memory alloys is investigated and a commonly observed hysteretic transformation is identified between a cubic $B2$ (austenite) structure and an orthorhombic $B19$ (martensite) structure.

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