Composition-property correlations in NiTi-based shape memory alloys from the first principles

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Abstract – Development of shape memory alloys (SMA) has been traditionally accomplished by means of extensive empirical efforts, with a very limited support from phenomenological models and related tools. We present a theoretical framework based on the Hamiltonian formalism, which connects important thermodynamic properties directly to the relative energies (the eigenvalues of the Hamiltonian), computed from the first principles using density functional theory. The estimates based on this formalism allow to establish correlations between composition and physical properties, such as relative energies, phase transition temperatures, hysteresis, thermal expansion, and other thermodynamic information. Importantly, estimates and correlations not only provide a fast answer, but also elucidate underpinning of thermodynamic features in terms of the electronic structure. Using this framework, we consider phase transformations and correlations between the selected properties and composition in the NiTi-based ternary and multicomponent shape memory alloys. Our theoretical guidance facilitates design and development of future alloys.

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