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Electronic mechanism of shape memory behavior in NiTi-based ternary alloys[1] N. HATCHER, A. J. FREEMAN, OLEG Y. KONTSEVOI, Northwestern University — While the electronic foundations of shape memory behavior in NiTi have been thoroughly examined and elucidated[2], we extend this understanding to ternary alloys. The effect of ternary additions on the martensitic behavior of NiTi is investigated by applying *ab initio* calculations with the highly precise FLAPW method to the Ni-Ti-X(X=Pt, Pd; 0-30%) system. We determine ternary element site preferences, pair interaction energies, and the energy hierarchy among the phases, finding that Pd and Pt atoms replace Ni and decorate the lattice at second and third nearest neighbors from one another, respectively. By calculating detailed elastic properties, cleavage energies, and planar generalized stacking fault energetics, we explain brittle/ductile behavior in the system, identify slip systems, and find that the C′ elastic constant becomes unstable with increased alloying. Finally, we establish how ternary elements affect the physics governing martensitic behavior by tracing changes in Fermi surface nesting behavior to mechanical instabilities and identifying unstable atomic vibration modes through imaginary branches of calculated phonon dispersions.

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[2]Hatcher, Kontsevoi, and Freeman, Phys. Rev. B,**79**, 020202(R) (2009)

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