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Electronic Structure Theory of the Structural Transformation of Shape Memory NiTi[1] NICHOLAS HATCHER, OLEG KONTSEVOI, ARTHUR FREEMAN, Northwestern University — The unique property of displacive phase transformations has created much interest in the study of martensitic materials. Among them, NiTi finds a wide range of applications due to its shape memory behavior; however, the detailed mechanism of its structural evolution during the martensitic transformation is not fully understood. We have investigated the transition paths between the B2, R, B19, and B19' phases using the highly-precise FLAPW method[2] to identify the governing processes of the transformation through calculations of the total energy, electronic structure, elastic moduli, and shear energetics. For example, we show the role of topological shifts of the Fermi surface and band structure evolution with the changing monoclinic angle of the B19' and R phases. In addition, the magnetism and magnetic susceptibility of the phases are investigated using both fixed spin moment and Stoner enhancement calculations. To date, we find the B2, B19, and B19' phases to be Stoner enhanced paramagnets.

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[2]Wimmer, Krakauer, Weinert, and Freeman, Phys. Rev. B, **24**, 864 (1981)

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