Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

New Transformation Path of Shape Memory NiTi[1] N. HATCHER, O. YU. KONTSEVOI, A.J. FREEMAN, Northwestern University — The detailed mechanism of structural evolution during the martensitic transformation in NiTi is not fully understood. To fully characterize the transformation path and to precisely determine the structure of its martensitic phase, we employ the highly-precise all-electron full-potential linearized augmented plane wave (FLAPW) method[2], and identify the governing processes of the martensitic transformations between the B2, B19, R, B19′ and recently proposed B33 and BCO phases. Several precursor phenomena for displacive phase transformations in the B2, B19, and R phases are identified, i.e. soft C_{44} and C' elastic constants, regions of Fermi surface nesting, and instabilities towards electronic topological transitions. By means of generalized stacking fault calculations, we find that the B2 phase has a low resistance to $\langle 100 \rangle \{110\}$ shear. A new, barrrierless transformation path from B2 to B19′ is established by calculating a bilayer $\langle 100 \rangle \{110\}$ shear with full structural optimization which leads to a monoclinic intermediate phase at 1/2a displacement; a relaxation of this structure's monoclinic angle results in the B19′ phase.

[1]Supported by AFOSR (grant # FA9550-07-1-0174).
[2]Wimmer, Krakauer, Weinert, and Freeman, Phys. Rev. B, **24**, 864 (1981)

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Date submitted: 29 Nov 2007 Electronic form version 1.4