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NiTi shape memory via solid-state nudge-elastic band[1] NIKOLAI A. ZARKEVICH, DUANE D. JOHNSON, Ames Laboratory — We determine atomic mechanisms of the shape memory effect in NiTi from a generalized solid-state nudge elastic band (SSNEB) method. We consider transformation between the austenite B2 and the ground-state base-centered orthorhombic (BCO) structures. In these pathways we obtain the R-phase and discuss its structure. We confirm that BCO is the ground state, and determine the pathways to BCO martensite, which dictate transition barriers. While ideal B2 is unstable, we find a B2-like NiTi high-temperature solid phase with significant local displacement disorder, which is B2 on average. This B2-like phase appears to be entropically stabilized.

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