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Martensitic phase transitions at the atomic length scale: Titanium Alpha to Omega[1]

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Martensitic phase transitions—diffusionless, first-order structural transitions occurring near the speed of sound—are abundant in both nature and technological applications from the earth's core to steels to shape memory alloys. Of particular interest to the aerospace industry are titanium alloys. However, pure titanium transforms under pressure to the brittle omega phase, a transformation that must be suppressed for technological applications. The theoretical understanding of this transformation involves finding the atomic pathway of the martensitic transformation. A systematic approach generates all possible pathways; they are successively pruned by energy estimates using elastic theory, tight-binding and *ab initio* methods. This general method reduces one thousand possibilities down to seven, and finally to the lowest energy pathway[2]. The lowest energy barrier pathway has a barrier four times lower than all others, and remains the lowest even when nucleation effects are considered. Molecular dynamics simulates the mobile interfacial boundary, and shows the transformation occuring at a fraction of the speed of sound. The resulting microscopic picture provides the starting point for understanding the effect of impurities and for the alloy transformations.

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[2]D.R. Trinkle *et al.*, Phys. Rev. Lett. **91**, 025701 (2003).