

Modeling the hcp to omega Phase Transition in Titanium.

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The equilibrium phase diagram of titanium contains two different hexagonal phases: hexagonal closed-packed (hcp) and the high-pressure omega phase[1]. While the pressure induced transition between these phases is known to be martensitic, the microscopic mechanics remains a mystery. Several models have been proposed, but connecting these to experiment—through orientation relations—has not identified a preferred mechanism. To elucidate this, we calculate the energy barrier of several possible pathways to determine the mechanics. Our simulations also allow us to understand the role of geometric effects in the microscopic pathway. Calculations were performed using a tight-binding model[2] that was refit for titanium to accurately reproduce the structural energies in a FPLAPW calculation, with a short-range functional form designed for use in molecular dynamics.

[1] S. K. Sikka, Y. K. Vohra, and R. Chidambaram, *Prog. Mater. Sci.* 27, 245-310 (1982).

[2] Michael J. Mehl and Dimitrios A. Papaconstantopoulos, *Phys. Rev. B* 54, 4519-30 (1996).