

Martensitic Phase Transitions in Titanium at the Atomic Length Scale

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Pure titanium transforms under pressure to the brittle ω phase, a transformation that must be suppressed for technological applications. Impurities greatly affect this transformation, for example, as little as 1% oxygen in commercial Ti alloys suppresses it. The theoretical understanding of this suppression involves two steps: (1) finding the atomic pathway of the martensitic transformation in pure titanium and (2) using this pathway that traps the impurities to estimate their effect. A systematic approach generates all possible pathways; they are successively pruned by energy estimates using elastic theory, tight-binding and *ab initio* methods. This last method reduces seven possibilities to the lowest energy pathway [1]. The speed of the diffusionless martensitic transformation traps dilute impurities, providing candidate pathways for alloyed materials. *Ab initio* refinements yield the change in both the relative stability of and the energy barrier between the phases due to impurities. The resulting microscopic picture explains the suppression of the transformation in the commercial Ti alloys Ti-6Al-4V and A-70 Ti [2].

References

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