

[1] D.R. Trinkle, R.G. Hennig, S.G. Srinivasan, D.M. Hatch, M.D. Jones, H.T. Stokes, R.C. Albers, and J.W. Wilkins, "A New Mechanism for the Alpha to Omega Martensitic Transformation in Pure Titanium," *Phys. Rev. Lett.* **91**, 025701 (2003).

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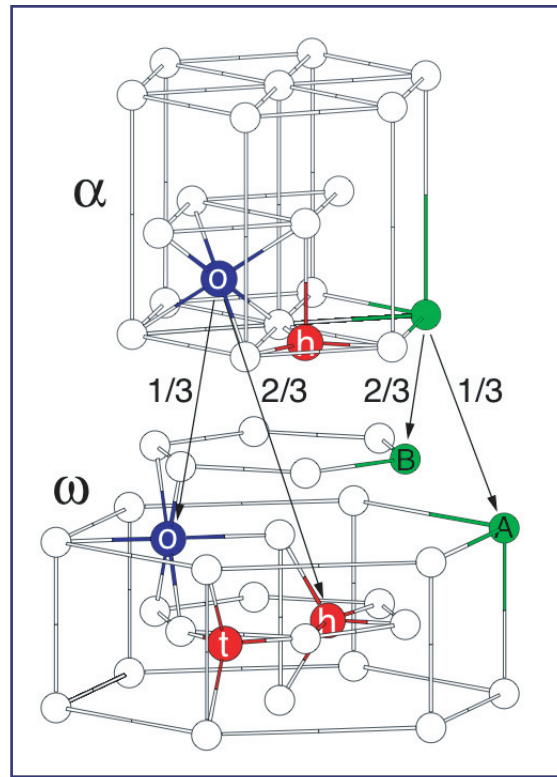


Figure 2— Impurity sites in α and ω . Octahedral (o), tetrahedral (t), and hexahedral (h) sites for interstitial impurities as well as A and B sites for substitutional impurities in the α and ω phases. The α and ω phases each contain one unique o, t, and h site. The α_{tet} site relaxes to the nearby α_{hex} site for all three impurities (O, N, C). The hexahedral site is a distorted double-tetrahedral site with five neighbors. The arrows indicate the transformation of the impurity and lattice sites in the TAO-1 mechanism [1] and the relative ratios. For clarity, the relative orientation of α and ω in TAO-1 is not shown.

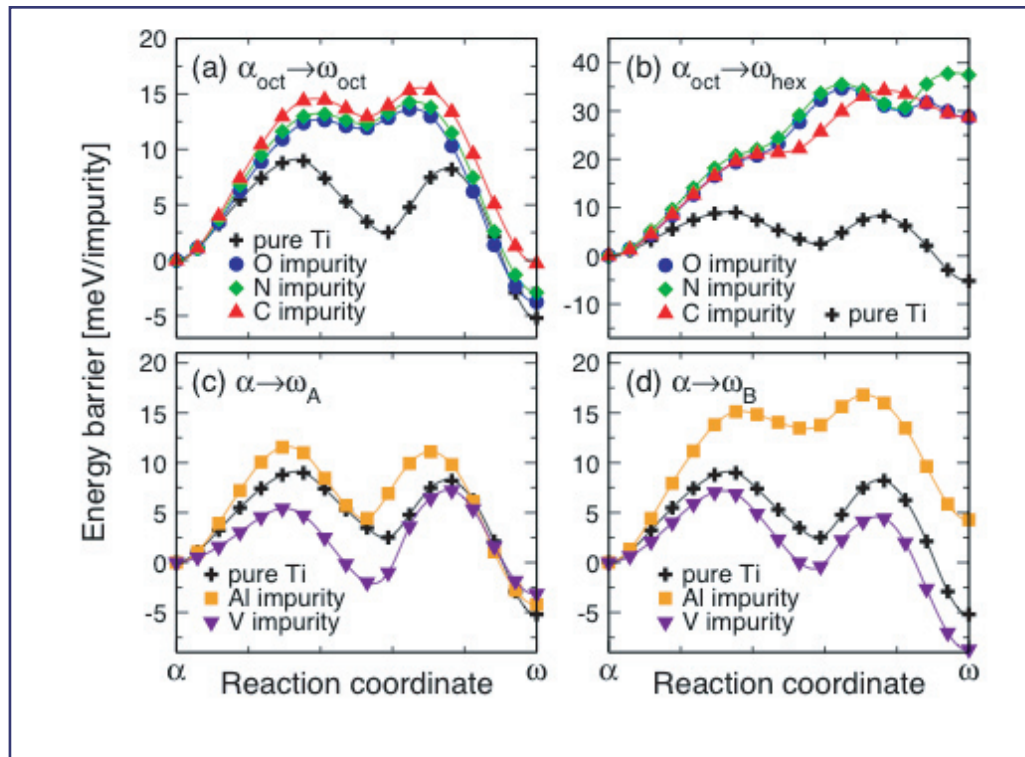


Figure 3— Impurities change the energy barrier of the $\alpha \rightarrow \omega$ transformation. The energy barriers for the TAO-1 transformation [1] of interstitial and substitutional impurities in Ti are shown relative to the α phase in units of MeV per impurity atom. The defect concentration is 2 at. %. The endpoint energies match the formation energies for a defect concentration of 1 at. % within 1 meV/atom, providing an accuracy estimate for the barrier. The interstitial O, N, and C impurities occupy the α_{oct} and transform into either (a) ω_{oct} or (b) ω_{hex} , with a 1:2 ratio. The substitutional Al and V impurities transform in ω to either (c) the A site or (d) the B site, with a 1:2 ratio.