

Structural similarities between Ti metal and titanium oxides: implications on the high-pressure behavior of oxygen in metallic matrices

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Abstract

The stabilities of the body-centered-tetragonal and distorted-diamond phases of titanium are investigated by first-principles methods. Our results, together with previous experimental and theoretical work, confirm two interesting observations. First, that the metal arrays in oxides correspond to stable or metastable phases of the parent metal; and second, that oxygen provides the pressure medium that stabilizes these phases. In addition, we have confirmed that the bulk modulus of oxygen matrices follows a nearly universal behavior with pressure, and that pressure-induced phase transitions tend to occur when the compressibility of the oxygen matrix reaches the compressibility of the high-pressure phase of the oxide.

Keywords

Titanium; Titanium dioxide; High pressure; Phase transformations; Density functional theory calculations