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Quantum-Mechanical Investigations for the Oxidation Mechanism of Ti_3Al WENHUA XUE, The University of Tulsa, SHI-YU LIU, Tianjin Normal University, SHIYANG LIU, Zhejiang Normal University, DEJUN LI, Tianjin Normal University, TARA DRWEN-SKI, SHUXIA YIN, SANWU WANG, The University of Tulsa — First-principles density-functional theory and thermodynamics calculations are combined to establish a microscopic mechanism for the oxidation of the α_2-$Ti_3Al(0001)$ surface. The surface energies as functions of the chemical potentials, as well as structural relaxations and electronic densities of states, are determined. The surface phase diagram (SPD) of the α_2-$Ti_3Al(0001)$ systems with different defects and at various oxygen coverages is constructed. It is found that the Al antisite defect prefers to segregate on the α_2-$Ti_3Al(0001)$ surface and oxygen adsorption enhances the segregation with the formation of the surface with three Al antisites per unit surface cell (i.e., the top surface layer is full of Al atoms) at the initial stage of oxidation, accounting for the aluminum selective oxidation observed experimentally. After the initial stage of oxidation, the O/α_2-$Ti_3Al(0001)$ system manifests itself with a non-uniform double-phase SPD, suggesting the competition between oxidations of the Al and Ti elements in the oxidation process. This result explains the experimentally observed second regime of oxidation in which both metal elements are oxidized.

Wenhua Xue
The University of Tulsa

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