First-principles Study on Surface Stability of Tantalum Carbides

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First-principles Study on Surface Stability of Tantalum Carbides

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ABSTRACT

Using first-principles method, surface energies of crystal planes of different tantalum carbide phases have been calculated. Quantum size effects are shown to possibly play a considerable role in determining accurate surface energies of these metallic films, which have been neglected in previous works. The γ-TaC phase has a more stable (0 0 1) surface than the close-packed (1 1 1) surface. In the α-Ta_2C phase, (0 0 1) surface with only Ta termination is more stable than that of mixed Ta-C termination, because the metallic bonds between Ta atoms are weaker than the Ta-C covalent bonds. The same is true for the ζ-Ta_4C_3 phase. The introduction of structural vacancies in the ζ-Ta_4C_{3-x} phase creates more direct Ta metallic bonds, making the Ta terminated surfaces even more stable. This is consistent with the experimental observations of cleavage of the basal planes, lamellae bridging of cracks, and the high fracture toughness of ζ-Ta_4C_{3-x}.

Keywords: First principles, Surface energy, Transition metal carbides

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