Physics of surface carbon ceramics by laser nanosrucTurization with 5d-metal componentry

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The carbon ceramics, such as titanium carbide (TiC) have attracted considerable interest as potential materials for nuclear reactors, aerospace application, and electronic devices due to its unique properties. In this paper, we systematically investigate the atomic structure, electronic and thermodynamic properties of adsorbed tungsten atoms on the polar Ti-terminated TiC(111) surface with different configurations of adsorptions using first principle calculations. The bond length, adsorption energy, and formation energy for different nanoreconstructions of the atomic structure of the W/TiC(111) systems were established.

The effect of tungsten coverage on the electronic structure and the adsorption mechanism of tungsten atom nucleation on the TiC(111) are also investigated. We also suggest the possible mechanism of tungsten nucleation on the TiC(111) surface. The effective charges on tungsten atoms and nearest-neighbor atoms in the examined reconstructions were identified. Additionally we have established the charge transfer from titanium atom to tungsten and carbon atoms, which determine by the reconstruction of the local atomic and electronic structures. Our calculations showed that the charge transfer correlates with the electronegativity of tungsten and nearest-neighbor atoms. We also determined the effective charge per atom of titanium, carbon atoms, and neighboring adsorbed tungsten atom in different binding configurations. We found that, with reduction of the lattice symmetry associated with titanium and carbon vacancies, the adsorption energy increases by 1.2 times in binding site A of W/TiC(111) systems.

Our results show that the nucleation of tungsten on the polar TiC(111) surface can be realized by three reconstruction mechanisms, which are responsible for the change in physical properties of material.

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