Microscopic Theory of Wetting and Adhesion in Metal-Carbonitride Systems

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Abstract

Joints between metals and ceramics are increasingly important in the manufacturing of many high technology products, from microelectronic devices to cutting tools. Wetting of ceramics by metals is the driving force of metal-ceramic joining processes, such as brazing and sintering of WC-Co cemented carbides and TiC-Co cermets. Experimental studies suggest that wetting in metal-ceramic systems is most sensitive to microscopic factors, like local chemical composition at interfaces.

This thesis is a theoretical study of the key microscopic mechanisms behind the wetting and adhesion, at the level of interatomic interactions. The ceramic materials considered are transition metal carbides and nitrides. The theoretical analysis is based on the results of first-principles density-functional calculations for a broad variety of model interface systems, using the plane-wave pseudopotential method. To deal with the problem of disordered interface structure, an approach based on comparative analysis of high-symmetry model systems is proposed.

It is demonstrated that the dominating mechanism of the Co/Ti(C,N) interface adhesion is a strong Co-C(N) bond. The number of those bonds is determined by an interplay of the interface incoherence and the structure relaxation effects. The particular strength of the Co-C bond is explained in terms of interface-induced features of the electronic states, in particular a novel metal-modified covalent bond. The obtained strength of the Co/TiC adhesion is in good agreement with available data from wetting experiments with liquid Co on TiC surface.

It is found that the Co ferromagnetism gives a significant change of the Co/TiC adhesion strength and interface energy, which is expected to be important during the solid-state sintering stage of the hardmetal manufacturing process. This effect can be adequately described within the Stoner model of itinerant ferromagnetism.

The known fact of better wetting in WC-Co systems than in TiC-Co ones is confirmed and explained in terms of a larger contribution of the metal-metal Co-W bonding at Co/WC interfaces.

The large scattering of the experimental wetting data for Cu and Ag on TiC and TiN is interpreted in terms of the different relative contributions of the elementary local atomic coordinations at the metal/Ti(C,N)(001) interfaces. Wetting is shown to be improved by C(N) vacancies and Ti segregation in the melt, in agreement with experimentally observed wettability improvements for hypostoichiometric carbides. The suggested simple microscopic picture of wetting in terms of different chemical bonds across the interface is also applied to the analysis wetting trends for Cu on HfC, ZrC, TaC, NbC, and VC.

Keywords: metal-ceramic interfaces; structure; bonding; wetting; adhesion; interatomic interactions; total energy and electronic structure calculations; density functional theory; carbides and nitrides; cermets; composites; hardmetals; sintering; brazing;