ID: P2.1

Title: Theoretical Study of Co/WC Interfaces

Name: Melnikov, Vladlen

Affiliation: Tomsk State University, Russia

Tungsten carbide is widely used in technological and industrial applications owing to its mechanical characteristics, high hardness, melting temperature, corrosion resistance. WC-Co composites have a unique combination of hardness and toughness thereby extending application field of the materials. Composite mechanical characteristics depend on physical and chemical properties of formed metal-ceramic interfaces which are defined by atomic and electronic structure of the interfaces as well as the metal and ceramic lattice mismatch. Since phenomena at the interfaces are vital for many technological processes they have been rather intensively studied last years. At the present work a theoretical investigation of atomic and electronic structure of differently oriented Co/WC interfaces is carried out within the density functional theory using the generalized gradient approximation for the exchange-correlation functional. The surface and the interface energies as well as the ideal adhesion energy of metal-carbide interfaces are estimated. The structural and electronic properties of the interfaces are discussed. The density of states peculiarities of interface atoms versus the orientation and structure of metal films are analyzed. The most stable film configurations on the tungsten carbide surfaces are found. The metal films chemical bonding characteristics at differently oriented interfaces are discussed. A relationship between electronic, geometrical factors and mechanical properties of the interfaces under study is analyzed. Obtained results are found to be in a good agreement with available theoretical and experimental data. Financial support was partly provided by the Russian foundation for basic research under grant No. 09-03-00523-a. Computational resources for this research were provided by the Interregional computational centre of the Tomsk State University (SKIF-Cyberia).