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Theoretical adhesion strength of diamond coating with metallic interlayers. HAIBO GUO, University of South Carolina, YUE QI, Materials and Processes Lab, GM R&D Center, XIAODONG LI, University of South Carolina — Metallic interlayers are often needed to enhance the adhesion of diamond coatings to substrates and to promote diamond nucleation and growth. The interfaces between diamond coatings and metallic interlayer materials with different carbide formation enthalpies, Cu, Al, and Ti, are studied using density functional theory. The ideal interface strength or the work of separation is found to decrease with the carbide formation enthalpy. Analysis to the electronic structure shows that covalent metal-carbon bonds form at the interface, and the perturbation from the interface weakens nearby metal phase. Comparing the work of separation at the interface with the fracture energy of the metal, a fracture is likely to initiate in the metal phase near the interface, therefore a tough metal with a large surface energy is needed to achieve a higher overall toughness. In addition, when the surface energy is larger than the interface energy, a wetted diamond/metal interface is formed during diamond nucleation, which also contributes to good adhesion. The interface energy, which is an energy barrier to diamond nucleation, is found to decrease with the carbide formation enthalpy. These results indicate strong carbide formability and a large surface energy of the interlayer enhance the adhesion and the fracture resistance of the interface, and also conduce to the diamond nucleation on the interlayer.

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