Atomistic Simulations of Interfacial deformation and bonding mechanism of Pd-Cu Composite Metal Membrane using Cold Gas Dynamic Spray Process.

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Abstract

The creation of atomic structures and the study of the deformation processes through molecular dynamics simulations have shown many advantages. However, gaps associated with the development and evolution of microstructure in the coating zone and dynamic processes that take place during cold gas dynamic sprayed materials still exist. The focus of this study was to investigate the interfacial deformation behaviours and the mechanism of bonding between atoms of palladium (Pd) and copper (Cu) composite metal membrane (CMM) using molecular dynamic simulations. The results confirmed that asymmetric deformation occurred during cold gas dynamic spray at the Pd-Cu interfacial region. As

the impact time increases, the layer thickness at the interface also increases. The concentrations of Pd-Cu CMM at the interfacial zone showed the presence of phase transitions at relatively long impact time. Furthermore, CGDS deformation was found to be an unsteady and dynamic process. Explicit bond analysis in this study also has shown that breaking of atomic bonds is not the key mechanism for the initial Pd□Cu plastic deformation occurrence. The higher interfacial bonding energy and interfacial shearing strength at the Pd-Cu CMM interface expressed the bonding strength and compatibility of Pd and Cu. Keywords: Molecular dynamics; CGDS; shear plastic-deformation: Bond mechanism