8th International Conference on Physical and Numerical Simulation of Materials Processing (ICPNS)

14–17 October 2016

Seattle, Washington | Hosted by Purdue University

SESSION 8: POSTER, GRAND PACIFIC BALLROOM
SUNDAY, OCTOBER 15, 2016

Microstructure and mechanical property of TiC/VC multilayered coatings from first principles

Tianmo Liu, Chongqing University

ABSTRACT

We have conducted a comprehensive first-principles investigation of tensile and fracture process of the TiC/VC interface by focusing on the strain–stress relationships, the ideal tensile strength, and bonding breaking process. The deformation analysis reveals that all bonds are extended at the initial stage until the critical point of fracture is reached. The fracture occurs between the second and third layers on the VC side in both (111) and (001) interfaces and the interaction of potential bonds of facture weakens gradually with the increment of strain during the tensile process. By using several analytical techniques, we identify a charge transfer in both the TiC and VC layers near to interface at the points of fracture during the tensile process, which plays a crucial role in affecting the fracture process. We further demonstrate that the fracture of the TiC/VC interface occurs within the VC and that adhesion energy cannot be simply used to represent tensile strength.

KEYWORDS: TiC/VC interface, adhesion energy, bonding nature, first-principles calculations