Molecular Dynamics Simulation of Impact of Palladium Clusters on the Zirconium Substrate[1]

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Abstract—Impact of palladium clusters with different sizes on a zirconium surface at various incident velocities was investigated by molecular dynamics simulation at the room temperature. The impact process was characterized by impacting of the cluster on the surface, intermixing and relaxation of the cluster and substrate atoms. Furthermore, the deformation compression ratio, flattening ratio and embedding depth of the palladium clusters were examined. Additionally, one region of the substrate surface impacting by the cluster was defined to study the evolution of the local surface temperature and stress with time during the impact process. It is found that the penetrating atoms of palladium clusters almost diffuse from the central area to the edge with increasing the collision velocity due to the ultrahigh hardness of the zirconium substrate. Compared to the lower incident velocity, the cluster with a higher incident velocity could generate much stronger shear stress. When the impact velocity reached up to 1100 m/s, the local temperatures was not high enough to melt the zirconium substrate. The local shear stress and heating promoted the combination between the cluster and substrate, but the local melting of the substrate does not emerge.

Keywords: molecular dynamics simulation, compression ratio, flattening ratio, local surface temperature, local shear stress.

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