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Molecular dynamics analysis of thermodynamic and kinetic properties of surfaces and interfaces of PdHx

This work uses molecular dynamics simulations to study surface and interface properties of PdHx that are relevant to hydrogen storage applications. In particular, surface energies, interfacial energies, surface diffusivities, and surface segregations are all determined as a function of composition and temperature. During the course of the calculations, we demonstrated robust molecular dynamics methods that can result in highly converged finite temperature properties. Challenging examples include accurate calculations of hydrogen surface diffusivities that account for all possible atomic jump mechanisms, and constructions of surface segregation composition profiles that have negligible statistical errors. Our robust calculations reveal that the Arrhenius plots of hydrogen surface diffusion is ideally linear at low compositions, and becomes nonlinear at high compositions. The fundamental cause for this behavior has been identified. This nonlinear surface diffusion behavior is also in good agreement with available experimental data for bulk diffusion. The implication of our calculated properties on hydrogen storage application is discussed.

Biography

X W Zhou completed his PhD from Clemson University, South Carolina, USA. He has been Principal Member of technical staff, Mechanics of Materials Department, Sandia National Laboratories since 2012. He has published more than 100 papers in reputed journals and has been serving as an Editorial Board Member of Journal of Materials Science Research.

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