DE LA RECHERCHE À L'INDUSTRIE

Séminaire

Lundi 14 septembre 2015 à 10h30

Salle de réunion du SRMP – Bâtiment 520 - Pièce 109

Hydrides and Hydrogen Pipe Diffusion in Palladium: First Principles, Kinetic Monte Carlo, and Neutron Scattering

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Studying the fundamental behavior of hydrogen in metals, like palladium, requires a combination of computation and experimental techniques. In Pd, hydrogen occupies octahedral sites and dislocation cores, which act as nanoscale H traps--forming Cottrell atmospheres that are metal-hydride-like at low temperatures. Using a combination of first-principles methods with atomic and mesoscale modeling, we can model the formation of the atmosphere and low temperature nanoscale hydrides, while in situ inelastic neutron scattering and small-angle neutron scattering measure vibrational changes and hydrides dimensions at the nanoscale. To understand the dynamics of hydrogen at a dislocation core, we compute changes in kinetics for diffusion above and beyond the changes due to elastic strain. We use this data for kinetic Monte Carlo studies of hydrogen pipe diffusion at different temperatures, and compare with new quasielastic neutron scattering measurements for a direct measurement of hydrogen pipe diffusion in palladium.

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