学术报告

题　　目：Thermodynamic versus kinetic origin of Super Abundant Vacancy formation in Ni single crystals in presence of hydrogen

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报告摘要：It has been showed experimentally that the vacancy concentration increases significantly in metals exposed to hydrogen, which has major implications on the embrittlement processes. However, the origin of this phenomenon remains unclear. In particular, thermodynamic and kinetic origins have to be clarified for a better control of the defect formation, and, therefore, to ensure the security of engineering structures.

Here, we have conducted first principles calculations of insertion and diffusion's barriers Gibbs free energies to determine the solubility and the diffusion coefficient of H in Ni single crystals both in the bulk material and in the vicinity of a vacancy. We determine the total H solubility and the vacancy concentrations at thermodynamic equilibrium from the minimization of the free energy of the system expressed in the grand-canonical ensemble and we find that the total vacancy concentration at is too small compared to the conducted experiments. The implementation of a kinetic model to follow the evolution of mobile and trapped H atoms in the vicinity of a vacancy indicates that the H-vacancy complexes concentrations becomes larger that the value given by the thermodynamic equilibrium. This result suggests that the system switch into an out-of-equilibrium state where the development of internal stresses may lead to the SAV formation but also to the formation of vacancy clusters.

报告人简介：Arnaud Metsue is an associate professor at the university of La Rochelle in France since 2012. His research is dedicated to the hydrogen-metal interactions from atomic scale calculations and it is done at the Engineering Science Laboratory for Environment. He got his PhD in condensed matter physics in 2010 at the university of Lille. Then, he moved to the Geodynamics Research Center at Ehime University in Japan to study the effects of iron on the thermodynamic properties of $MgSiO_3$ phases.