DE LA RECHERCHE À L'INDUSTRIE

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Séminaire

SRMP

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Mean field modelling of interstitial transport in irradiated ferritic-martensitic steels

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Flux coupling between point defects and solute atoms is the key for understanding the formation mechanisms of embrittling nanofeatures in reactor pressure vessel steels. When solute-defect interactions are sufficiently strong, correlation effects can arise and a defect flux can lead to solute migration even in the absence of thermodynamic driving forces. In spite of their importance, such kinetic correlations are often disregarded in existing diffusion models for ferritic-martensitic dilute alloys.

In this work, an interstitial-mediated diffusion model is presented for six bcc iron-based dilute binary alloys respectively containing Cu, Mn, Ni, Cr, P and Si. The model is based on the combination of ab initio calculations of interstitial and vacancy jump frequencies with the Self Consistent Mean Field (SCMF) theory**,** for an exact calculation of transport coefficients (Onsager matrix). For this purpose, a Matlab code was successfully developed for the application of the SCMF theory to the problem of dumbbell-mediated transport in generic A-B dilute alloys. The aim of the project is on one hand to build a database of accurate migration barriers for ferritic steels, and on the other hand to detect correlation effects between defect and solute fluxes. The transport coefficients are also combined with the previously computed vacancy coefficients in order to predict radiation-induced segregation profiles.

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