DE LA RECHERCHE À L'INDUSTRIE

# Séminaire

## Mercredi 24 octobre 2012 10h30

**Salle de réunion du SRMP – Bâtiment 520 - Pièce 109**

# *Impurity diffusion and transport coefficients in dilute binary Fe-based alloys*


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Ferritic-martensitic RPV steels are subjected to radiation-induced embrittlement due to the formation of complex defect-solute clusters which hinder the dislocation motion. The latest surveillance tests on Swedish RPV samples have shown a sudden increase of the DBTT shift at high irradiation doses, which is most likely caused by the unexpected development of new clustering objects. The interactions of impurities with point defects play a key role in this process.

The object of this work was to analyze such interactions from the point of view of vacancy-mediated diffusion. Three different methods were used for computing the transport coefficient matrix: the 10-frequency model, the self-consistent mean field theory (SCMF) and Monte Carlo simulations. A set of vacancy-solute and vacancy-solvent migration barriers was computed ab-initio for dilute FeCu, FeMn, FeNi, FeCr, FeSi and FeP alloys. The results show that all the considered impurities interact strongly with vacancies and are expected to be involved in the vacancy wind mechanism, with the exception of Cr. The SCMF method proved also to give more accurate results than the more commonly used 10-frequency model.


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