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SEMINAIRE



Service de Recherches de Métallurgie Physique DEN/DANS/DMN

Salle de réunion du SRMP - Bâtiment 520 - Pièce 109

Nucleation of helium atoms in BCC iron studied by MD simulations

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Helium atoms generated via (n, α) reaction are considered to be one of the main reasons for the degradation of materials used in nuclear energy reactor systems. Through clustering He bubbles are formed leading to embrittlement. In this presentation, the nucleation of helium atoms in single crystal and the grain boundary systems studied by molecular dynamics (MD) simulations are given. The processes of athermal emission of self-interstitial atom (SIA) and the formation of dislocation loop by helium atoms in single BCC iron are firstly predicted. And furthermore, He-clusters in the symmetrical grain boundaries ($\Sigma 3\{111\}$, $\Sigma 3\{112\}$ and $\Sigma 5\{012\}$) and general nano-grain boundaries including the high, low angle and non-ideal (close to $\Sigma 3$) symmetrical grain boundaries are also investigated. The local atomic excess free volume (LAEFV) is found to be main parameter affecting the helium nucleation process in grain boundary system by comparing with results of helium in single crystal.

Lundi 20 Septembre 2010 à 10h30

N.B : *Les visiteurs de nationalité étrangère hors Union Européenne sont priés de bien vouloir avvertir impérativement 3 semaines à l'avance - les visiteurs de l'Union Européenne 1 ou 2 jours avant le séminaire - le Secrétariat du Service de leur entrée sur le Centre :*
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