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SEMINAIRE



Service de Recherches de Métallurgie Physique

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Salle de réunion du SRMP – Bâtiment 520 – Pièce 109

Modeling of Screw Dislocations in W-based Alloys

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Tungsten is currently considered as the divertor material in fusion reactors. However, the material undergoes a brittle to ductile transition above room temperature, which imposes severe constraints on the usability. This inherent brittleness is due to the relatively low mobility of the $\frac{1}{2}\langle 111 \rangle$ screw dislocation. It is, therefore, of great importance to understand its properties and the influence of alloying elements.

In this talk we will present ab-initio calculations, aiming to explore the influences of alloying elements on the $\frac{1}{2}\langle 111 \rangle$ screw dislocation of tungsten. We are particularly interested in the structure of the dislocation core and the critical stress needed to move the dislocation, i.e. the Peierls stress. We find that alloying with Re induces a change from a non-degenerate to a degenerate core and a reduction in Peierls stress consistent with the experimentally found solute solution softening and change in slip plane. These trends are not revealed by other alloying elements, such as Ta which retains a non-degenerate core and increases the Peierls stress at low alloying concentrations. As a last step we investigate potential correlations of these effects with more basic properties of the alloys such as elastic moduli or gamma surfaces.

Judi 24 mars 2011 à 10h30

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