Laboratoire des Solides Irradiés, UMR 7642

Soutenance de thèse

Vendredi 18 Mars 2016
Amphi Becquerel - 14h00

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Ab initio simulation of extended defects of α-Ti in presence of interstitial atoms H/O

This Ph.D. thesis has been devoted to the study of extended defects of α-Ti in presence of interstitial atoms H/O via ab initio simulation. It is divided into three parts. In a first part, the octahedral interstitial site of α-Ti is found energetically more favorable for a H or an O atom. The presence of H decreases the shear modulus G and Young's modulus E of α-Ti while O has an opposite and stronger effect. H increases the B/G ratio while O decreases it. In a second part two new stacking faults are found. A <c+a> screw dislocation 3-part dissociation mechanism is proposed and studied. The presence of O may make the stacking faults formation energetically more difficult, contrary to the H case. For the <a> screw dislocation, both H and O in core sites change the metastable gliding prismatic dissociation to π1 plane or to a prism-π1 plane mixed configuration. According to our measurements of Peierls energy barriers with O at different sites and concentrations, O makes the gliding much more difficult. Cross-slip should happen in that case. H segregates more strongly than O to <a> screw cores but has a slightly attractive interaction with O and is less present than O in Ti, which probably explains why the effect of H on the plasticity of α-Ti is a complex issue. In the last part, the {10-12} and {10-22} twin boundaries (TB) structures are shown to fail for deformations as low as 1% or 2% along the c-axis. The {11-21} and {10-11} TBs are much more resistant. The presence of segregated H and O enhances the {10-12} and {11-22} TB limited stability. A twinning disconnection (TD) dipole model is proposed and applied to the {10-12} case. Segregation energy calculations show that H and O should distribute more or less homogeneously to the TD core and the TB, with only a slight preference to the TD core although not at the interstitial sites of the atomic layer related to the disconnection step itself.

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