MASTERS INTERNSHIP REFERENCE : ST2116SC

Ab initio molecular dynamics simulations of SiC(*s*)/$Si_{1-x}B_x$(*l*) interfaces: understanding the stabilizing effect of boron

Context

Ceramic matrix composites (SiC/SiC) are key materials in current and next generation civil aircraft engines. The current deposition process of the matrix involves the melt infiltration of Si, which results in an important etching of SiC associated to the dissolution of some C within the liquid Si. Recent experimental results have shown that the introduction of boron within the melt significantly reduces this etching, yet, the details of this stabilization of the SiC(s)/Si(l) interface are not understood so far. A plausible hypothesis is that boron could segregate at the interface and form a stabilizing coating.

Aim & methods:

We propose here to perform some ab initio molecular dynamics (AIMD) simulations of SiC(s)/$Si_{1-x}B_x$ interfaces for various SiC surfaces (100, 110, 111) and B concentrations (x). Analysis of the AIMD trajectories should allow investigating the viability of the boron interface segregation hypothesis and, if confirmed, investigate the interface structure. Additionally, simulations of $Si_{1-x-y}B_xC_y$ liquids will be performed to determine the influence of B content on the self-diffusion coefficient of C atoms, a reduction of C mobility due to B being another possible explanation for the positive effect of B addition.

Techniques used :

Ab initio molecular dynamics simulations, density functional (tight-binding) theory, scientific coding for results analysis

Host lab : ISM & LCTS

Funding : Safran Ceramics

Duration: 5 to 6 months

Required profile : Skills in computational chemistry.

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