Helium Diffusion and Cluster formation in Iron-Chromium Alloy: A First Principle Molecular Dynamics Study

Introduction

Helium has a very low solubility in metals. Initially they form either helium clusters or complex & then diffuse and coalesce to form bubbles of nano-meter size or more. These bubbles are one of the reason for ferritic steel to be used in TBM to fail in brittle manner.

Atomic simulation needs to be carried out to gain a physical understanding of the phenomenon.

Tools and Technique

LAMMPS is used as a simulation code and OVITO & Paraview are used for visualization of atoms.

CrHe intenct potential developed by Caro et. al is used as input file in present work.

Overview of Work

Atomistic simulation of single helium and its cluster in Fe-10%Cr alloy is done. Study provides parameters in terms of helium diffusion, volume, energy and pressure at reactor working temperature.

Diffusion of single helium in bi-crystals of eight different orientation in the temperature range of 700 - 1000 K is presented.

Simulations on helium cluster with more than a thousand helium atoms at 800 K.

The inter-atomic potential used as input has been validated as shown in below table.

<table>
<thead>
<tr>
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<th>Obtained</th>
<th>Literature</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk Modulus (MPa)</td>
<td>173.8</td>
<td>168.6</td>
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<tr>
<td>VFE (eV)</td>
<td>1.81</td>
<td>1.63 - 2.05</td>
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Helium Diffusion Model

![Fig. 1(a). Path of Helium atom at 300 K and 800 K](image)

![Fig. 1(b). Path of Helium atom 800 K at grain boundary](image)

- A continuous pocket of trap site is seen at Grain Boundary (GB) which is reflected by decrease in Diff. Coeff. by an order of magnitude in GBs.
- Migration energy and pre-exponential factor of He diffusion in different orientations is also obtained.

Bubble Nucleation and Growth

- Helium cluster are known to block the motion of dislocation inside the materials.
- They also acts as a nucleating site for dislocations.
- First dislocation is emitted when cluster reaches a critical radius of 0.35 nm.

Helium Bubble Analysis

- Owing to the greater atomic packing fraction at 0.1 K, the helium atoms are more potentially unstable as compared to 800 K.
- The stress tensor acting on nearby host atoms forces the He bubble to grow in elliptical shape.
- Corresponding, radius and volume equation has been obtained.

- Potential energy of surface atoms is 0.1-0.15 eV higher than the bulk atoms.
- Helium bubble of 2.65 nm at 800 K, the width of surface atoms is nearly 0.9 nm, making up to the 30% of the overall radius of the bubble.

- The nucleation and emission of dislocation is observed by the energy relaxation of He atoms.
- Emission is more frequent for bubble size less than 1.5 nm radius.
- The pressure is dependant upon surface to bulk (S/B) atoms. For rho > 2, S/B is higher is pressure increases and vice versa.

Conclusion

- Diff. Coeff. of He in GB is an order of magnitude higher than bulk.
- For He bubble between size range of 1-2 nm, the pressure is ~40 - 20 Gpa, pe is ~ 0.4 eV. (Single He pe is 2.5 eV)

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References


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