Contribution ID: **263** Type: **Poster Presentation**

Investigation of S diffusion in bulk Fe – a DFT study

Wednesday, 13 July 2011 17:00 (2 hours)

<p>The diffusion of a dilute S solution in Fe was investigated in order to determine the diffusion path and the energy required, Q, for diffusion in a bulk Fe crystal structure. Different pseudotopotentials were investigated in order to determine the pseudotopotential that best describes the ground state of the bulk Fe structure. Pseudotopotentials that gave a good description of the ground state were subsequently tested to find the appropriate bulk cell size that will give the best description of S diffusion in Fe. This was done by calculating the binding energy of pure Fe and that of S in Fe for different cell sizes and to find the cell size were the binding energy converges. Using the appropriate cell size, an investigation was performed in order to determine the diffusion mechanism of S in Fe. The nudged elastic band method was employed to calculate the minimum energy path of S diffusion in Fe, which gives the energy required for diffusion of S in Fe, namely the activation energy, Q. Activation energies for both interstitial S and substitutional S in the Fe crystal was calculated by the nudged elastic band method in order to determine the most energetically favourable diffusion mechanism for S in bulk Fe.

Level (Hons, MSc,
   PhD, other)?

M.Sc

Consider for a student
   award (Yes / No)?

yes

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

yes

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