CLUSTERING OF HELIUM ATOMS AT A $\frac{1}{2}(111)\{110\}$ EDGE DISLOCATION IN $\alpha$-IRON


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(Received 5 June 1977 by A.R. Miedema)

Atomistic calculations on a $\frac{1}{2}(111)\{110\}$ edge dislocation show a restricted tendency of clustering of helium atom along this dislocation. Clusters with up to 4 helium atoms have been studied. A cluster with 3 helium proved to be most stable.

IN THIS COMMUNICATION results of atomistic calculations on helium clustering around a $\frac{1}{2}(111)\{110\}$ edge dislocation in $\alpha$-Fe are reported.

Binding of one helium atom to such dislocations in W and Mo has already been predicted in a previous communication [1], so has been the clustering of helium atoms in $\{110\}$ planes of a perfect lattice in Mo [2]. On the other hand it has been shown that clustering of C-atoms around a $\frac{1}{2}(111)\{110\}$ edge dislocation in $\alpha$-Fe is energetically not likely [3].

In view of the 6-layer periodicity of $\{112\}$ planes along the dislocation line the crystallite used in the atomistic calculations was composed of 13 of such planes, with the dislocation intersecting these planes through their midpoints. The total number of atoms in the crystallite was restricted to about 1400 in order to save computer time.

The anisotropic elastic theory developed by Eshelby et al. [4] was used to find the initial positions of the atoms in the crystallite (the elastic constants of Fe [5] do not satisfy the isotropic condition $C_{44} = (C_{11} - C_{12})/2$, thereafter the atoms were allowed to relax to minimum energy positions under the influence of interatomic pairwise central forces. To obtain these forces the Fe-Fe and He-Fe potential functions of Johnson and Wilson [6] * and of Wilson and Johnson [7] were used, respectively, and the He-He potential function of Abrahamson [8]. The first, second, 12th and 13th $\{112\}$ planes were allowed to move during relaxation as periodic boundaries, the other boundary planes of the crystal ($\{110\}$ and $\{111\}$) were kept fixed.

The relaxed positions thus obtained of the atoms in six adjacent $\{112\}$ planes are shown in Fig. 1 as projected on one another. To find possible positions where helium atoms could be bound to the dislocation the unrelaxed helium configuration energy $E_{\text{He}}^{\text{up}}$ was calculated for a grid of positions with one-tenth interplanar spacings within the volume PQRS indicated in Fig. 1. In these calculations the Fe-lattice around the helium atom was not allowed to relax. $E_{\text{He}}^{\text{up}}$ proved to have minimum values in the slip plane of the dislocation. Figure 2 shows how $E_{\text{He}}^{\text{up}}$ varies in this plane; within the volume (comprising six $\{112\}$ planes) six minimum energy valleys were found.

Subsequently a helium atom was placed in each of the minimum energy positions and the lattice was allowed to relax. The positions with the lowest energies thus determined are indicated in Fig. 2 as positions A, B and C, all having an energy of 3.36 eV.

Again in each of the three cases the $E_{\text{He}}^{\text{up}}$ value of a second helium atom was determined. After relaxing the lattice the pair $(A, D)$ appeared to be the most favourable one, having a configuration energy of 6.12 eV. The procedure was repeated for a cluster of three helium atoms, including the two helium atoms in sites $A$ and $D$. The third helium atom had a minimum configuration energy, when it is placed in $E$. Figure 3 shows the relaxed positions of these three helium atoms. For a cluster of four helium atoms the configuration ADEF was found. The results are given in Table 1 using the following notations:

| He    | = interstitial helium atom far from the dislocation. |
| D     | = dislocation. |

* This Fe-Fe potential function differs slightly from the Johnson I potential.
Fig. 1. The projected positions of atoms in six adjacent \{112\} planes relaxed around a \(\frac{1}{6}\) \{111\}\{110\} edge dislocation. The atom symbol used for each of the planes a, b, c, d, e is indicated. Dimensions are given in half lattice units (h.l.u.).

Table 1. Binding energies of He-clusters of \(n\) atoms around a \(\frac{1}{6}\) \{111\}\{110\} edge dislocation

<table>
<thead>
<tr>
<th>(n)</th>
<th>(E_{\text{HeD}_n}^F)</th>
<th>(E_{\text{HeD}_n}^{\text{He}})</th>
<th>(E_{\text{He}}^{\text{HeD}})</th>
<th>(E_{\text{He}}^{\text{HeD}_n})</th>
<th>(E_{\text{He}}^{\text{HeD}_n})</th>
<th>Configuration, see Fig. 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.36</td>
<td>2.10</td>
<td></td>
<td></td>
<td>3.90</td>
<td>(A, B) or (C)</td>
</tr>
<tr>
<td>2</td>
<td>6.12</td>
<td>2.70</td>
<td>0.60</td>
<td></td>
<td>2.42</td>
<td>(AD)</td>
</tr>
<tr>
<td>3</td>
<td>8.59</td>
<td>2.99</td>
<td>0.89</td>
<td></td>
<td>2.25</td>
<td>(ADE)</td>
</tr>
<tr>
<td>4</td>
<td>11.50</td>
<td>2.55</td>
<td>0.45</td>
<td>(___)</td>
<td>–</td>
<td>(ADEF)</td>
</tr>
</tbody>
</table>

* This value has been arbitrary taken 0.2 eV higher than the corresponding \(E^B\) value in view of our calculated value for \(E_{\text{He}}\) = 0.13 eV in a perfect lattice (Wilson and Johnson 0.17 eV [7]).

(HeD) = helium atom bound to the dislocation.
(HeD)_n = a cluster of \(n\) dislocation-bound helium atoms.
\(E^F\) = configuration energy, \(E^B\) = binding energy, \(E^M\) = migration energy and \(E^D\) = dissociation energy (\(=E^B+E^M\)).

The binding energy \(E_{\text{HeD}_n}^{\text{He}}\) in Table 1 is the one that is released in the reactions.

\[
\text{He} + D \rightarrow \text{(HeD)}, \\
\text{He} + (\text{HeD})_n \rightarrow (\text{HeD})_n, \quad n = 1, \ldots 
\]

So \(E_{\text{HeD}_n}^{\text{He}} = -E_{\text{HeD}_n}^F + E_{\text{HeD}_n-1}^F + E_{\text{He}}^F\) with \(E_{\text{He}}^F\) being the \(E^F\) of interstitial helium in a perfect lattice.

For this value we found 5.46 eV, (Wilson and Johnson 5.36 eV [7]). \(E_{\text{HeD}_n}^F \equiv E_n^F\) is the \(E^F\) value of the dislocation without helium attached to it.

The binding energy \(E_{\text{HeD}_n}^{\text{HeD}}\) refers to the reaction

\[
(\text{HeD}) + (\text{HeD})_{n-1} \rightarrow (\text{HeD})_n, \quad n = 2, 3, \ldots
\]

with \(E_{\text{HeD}_n}^{\text{HeD}} = -E_{\text{HeD}_n}^F + E_{\text{HeD}_n-1}^F + E_{\text{HeD}}^F\).

The reaction assumes that a (HeD) can migrate along the dislocation and thus can meet another (HeD)_n cluster or (HeD). The migration energy of a (HeD) along a dislocation has not been determined but can be expected (with reference to the corresponding value of \(\sim 0.4\) eV found for Mo and W [1]) not to be higher than the value \(E_{\text{HeD}}^F \approx E_{\text{He}}^F + E_{\text{He}}^M\).
In other words, a dislocation-bound helium atom will migrate along the dislocation sooner than release itself from the dislocation.

The numbers in Table 1 make it clear that — unlike carbon atoms [3] — helium atoms do tend to cluster with increasing binding energy $E_{\text{HeD}}$ along an $\frac{1}{4}(111)\{110\}$ edge dislocation in $\alpha$-Fe. The tendency is, however, restricted as indicated by the reduction in binding energy of the fourth ($\text{HeD}$). It should further be noted that this cluster tendency will not lead — in a desorption experiment — to higher release temperatures since the ($\text{HeD}$) cluster will first dissociate via reaction (2) into separate ($\text{HeD}$)'s which will then dissociate from the dislocation with an activation energy $E_{\text{HeD}} \approx 2.3$ eV. If a migrating ($\text{HeD}$) will be able to reach a jog in the dislocation it will be more strongly bound. In this respect the calculated dissociation energies of helium from a monovacancy are of interest (last column in Table 1). At such a jog the cluster tendency will be most likely enhanced. Further work will include helium clustering at dislocation jogs.

Fig. 2. Result of the $E_{\text{HeD}}$ values calculated for a grid of positions within the volume PQRS indicated in Fig. 1. Open and filled circles indicate atoms just above and below the slip plane. Positions of minimum energy along $(-1, 1, 1)$ directions, connected by the drawn lines, appear to be in the slip plane. The squares and crosses indicate minimum and maximum energy positions along the drawn lines. For positions A B C D E see text.

Fig. 3. Three clustered helium atoms ($A, D, E$) in the core of the $\frac{1}{4}(111)\{110\}$ dislocations. Relaxed positions of atoms in planes just above and below the slip plane are shown. Dimensions are given in half lattice units.
REFERENCES