**Ab initio** modelling of Y-O complexes in α-Fe matrix

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**Abstract**

ODS (Oxide-Dispersion-Strengthened) steels with Y:O are promising materials for structural applications in future nuclear fusion reactors. The great amount of experimental research has been made so far. However, many details of the Y:O nanoparticles’ behaviour at the very atomic level still remain unclear. For better understanding of the mechanics and kinetics of the ODS particle formation process, we have performed theoretical modelling. We have applied the Density Functional Theory (DFT) method, as implemented in the computer code VASP. The initial step has been chosen to simulate the Y-O complexes in the α-Fe matrix. Various configurations of yttrium and oxygen solute atoms, combined with vacancies have been investigated. Acquired from these calculations data will be used as an input for the further kinetic Monte Carlo simulations.

**Keywords:** ODS, DFT, VASP

**1 Introduction**

The study of ODS (Oxide-Dispersion-Strengthened) steels is important because of their ability to withstand high neutron radiation at relatively high temperatures (650°C) [1] which makes them suitable material for building the first wall of future nuclear reactors.

In this paper we present the initial step of theoretical modelling of the behavior of ODS nanoparticles in α-Fe (or bcc-Fe) matrix. The study of α-Fe is of a particular interest, since this phase of iron corresponds to the operation conditions. We perform ab-initio calculations for different configurations of yttrium and oxygen solute atoms, combined with vacancies.

**2 Computational details**

All calculations in this study have been performed using the computer code VASP (Vienna Ab-initio Simulation Package) [2] which implements plane wave basis set and DFT (Density Functional Theory) method.

The generalized gradient approximation (GGA) ultra-soft (US) projector augmented wave (PAW) Perdew-Burke-Ernzerhof (PBE) pseudopotentials (PP), provided by VASP developers, were used for each element.

The supercell with the size of 4x4x4 elementary cells has been used. According to convergence test, both the k-mesh size 4x4x4 and plane wave energy cutoff 450 eV are sufficient to achieve the goal of this study.

**3 Simple Defects**

By simple defects we mean single point-like defects of yttrium and oxygen as well as some their combinations with vacancies. The calculated vacancy formation energy is 2.16 eV, which qualitatively corresponds to results of other theoretical and experimental studies [3].

In the Table 1, the energies for different configurations are provided, relatively to the minimal energy of the investigated configurations.

Despite the non-negative energy of the vacancy formation energy, \( V_{\text{Fe}} - Y - V_{\text{Fe}} \) configuration still has a lower energy, which means that we need vacancies in the matrix in order to attract yttrium atoms inside the system.

The system with oxygen in the substitutional position also has the lowest energy, however, as it is shown in the section 5, oxygen in octahedral position 1NN away from the vacancy possesses a significantly lower energy.

**4 Energy Barriers between Simple Defects**

It is also important to calculate the energy barriers, between simple defects by estimating the minimal energy path (MEP) with nudged elastic band (NEB) method with climbing.

The calculated heights of barriers for vacancy migration in the [111] and [100] directions have been found to be 0.7 eV and 2.6 eV, respectively. Since the difference between \( O_{\text{oct}} \) and \( O_{\text{tet}} \) is fairly small, we have calculated the barrier between them. It has appeared that \( O_{\text{tet}} \) is almost a saddle point itself for the transition \( O_{\text{oct}} \rightarrow O_{\text{oct}} \) with the height 0.42 eV.

Also, the height of the barrier for a jump of yttrium atom from one vacancy to another in the direction [100] is appeared to be fairly low: 0.44 eV.

**5 Complex Defects**

As complex defects, we consider different combinations of the simple defects. We have calculated the interaction energies in the following systems: \( V_{\text{Fe}} - O_{\text{oct}} \), \( V_{\text{Fe}} Y V_{\text{Fe}} - O_{\text{oct}} \), and \( V_{\text{Fe}} Y V_{\text{Fe}} - 2O_{\text{oct}} \).

**Table 1** Energies of the configurations with simple defects, energy is given relatively to the minimal energy in the column.

<table>
<thead>
<tr>
<th>System with Y</th>
<th>Energy, eV</th>
<th>System with O</th>
<th>Energy, eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_{\text{Fe}} - Y - V_{\text{Fe}} )</td>
<td>0.00</td>
<td>( O_{\text{tet}} )</td>
<td>0.00</td>
</tr>
<tr>
<td>( Y_{\text{tet}} )</td>
<td>1.35</td>
<td>( O_{\text{oct}} )</td>
<td>0.58</td>
</tr>
<tr>
<td>( Y_{\text{oct}} )</td>
<td>9.76</td>
<td>( O_{\text{oct}} )</td>
<td>1.00</td>
</tr>
<tr>
<td>( Y_{\text{oct}} )</td>
<td>16.41</td>
<td>( \text{Fe-O}_{\text{Fe}} )</td>
<td>3.01</td>
</tr>
</tbody>
</table>

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It is also important to calculate the energy barriers, between simple defects by estimating the minimal energy path (MEP) with nudged elastic band (NEB) method with climbing.

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signifies that we should put oxygen in octahedral position in more complex configurations.

The results for $V_{Fe}$-$Y_{Fe}$-$O_{oct}$ are shown in a Figure 2. The most stable configuration is found and also it is shown that $V_{Fe}Y_{Fe}$-$O_{oct}$ (1NN) is a metastable configuration and relaxes to the most stable if the symmetry of the system is broken.

The different configurations $V_{Fe}Y_{Fe}$-$2O_{oct}$ have been created by adding a second $O_{oct}$ to the most stable $V_{Fe}Y_{Fe}$-$O_{oct}$ configuration. The results are displayed in the Figure 3. We still can notice that if oxygen is 2NN away from yttrium substitute, the configurations tend to be more stable.

6 Conclusions

Various configurations of yttrium and oxygen solute atoms, combined with vacancies, have been thoroughly investigated.

To continue the research, we need to calculate the barriers between more complex configurations before we proceed with the kinetic Monte Carlo simulations.

Acknowledgments

All the calculations have been performed using the “Helios” supercluster (Japan).

References