**Ab initio** calculations of Y, O and $V_{Fe}$ migration barriers inside fcc-Fe lattice

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Abstract

Using results of density functional theory (DFT) calculations the first attempt towards the understanding of $Y_2O_3$ particles formation in oxide dispersed strengthened (ODS) ferritic–martensitic steels has been performed. The present study includes modelling of single defects (O impurity atom, Fe vacancy, $V_{Fe}$, and Y substitute atom), interactions between $Y-Y$, $Y-V_{Fe}$, $Y-O$, $V_{Fe}-V_{Fe}$ and O-O pairs inside the fcc-Fe matrix, as well as more complicated defect structures. Calculations of Y and O atom migration paths inside iron matrix have been performed using the Nudge Elastic Band method.

**Keywords:** ODS steels, O and Y precipitates, Fe vacancies, density functional theory

1 Introduction

Reduced activation ferritic-martensitic steels (RAFM) strengthened by oxides provide a growth of the operating temperature for the future fusion and advanced fission reactors by 100°C up to 650°C or even higher. $Y_2O_3$ is the most commonly used oxide for the strengthening of RAFM steels as it is one of the most stable oxides with melting temperature higher than that of the steels, which might play significant role in the formation of oxide nanoparticles in (ODS) steels. They are produced by mechanical alloying for several tens of hours, followed by a hot isostatic pressing (hipping) at temperature around 1000-1200°C and pressure ~100 MPa. Experimental evidences suggest that a significant part of yttrium and oxygen atoms were observed in steel matrix with concentrations above their equilibrium solubility. This might mean that precipitation of $Y_2O_3$ nanoparticles occurs already during the hipping stage.

2 General

A slow diffusion of large yttrium-substituted atoms is probably the major limiting factor for $Y_2O_3$ particle growth. The diffusion of interstitial oxygen is much faster and, therefore, cannot delay the growth of precipitates significantly. That is the reason why our calculations are focused on the study of the migration properties of $Y-V_{Fe}$ complexes and the role of $V_{Fe}$ vacancies as well as oxygen impurity atoms in yttrium-yttrium binding.

In this study, we have performed extensive DFT-PAW (Projected Augmented Wave) calculations of elementary yttrium and oxygen complexes inside the iron lattice containing also $V_{Fe}$ vacancies in both 4x4x4 and 5x5x5 Fe supercell models using PW91 Hamiltonian as implemented within VASP code [1-3]. Both interaction energies between solute and matrix atoms and barriers for migration of different solute atoms are extracted from these calculations for further atomistic simulations.

Binding energies between the impurity atoms and vacancies as well as their migration barrier energies are important parameters for further LKMC modeling of the ODS particle formation.

3 Conclusions

To perform calculations on migration barriers of atms inside the lattice, the nudge elastic band (NEB) method have been used (as implemented within the VASP computer code). The calculations of different Y migration trajectories have been performed. The lowest calculated energy of the migration barrier has been found to be about 1.75 eV. The high values of migration energies prove that the increased concentration of vacancies is required for Y diffusion and the increased size of the supercell is required for this purpose.

References