

First Principles Simulations on Yttrium, Oxygen, and Titanium Precipitation inside *fcc*-Fe Lattice

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Abstract

The detailed modeling of the defect in the face centered cubic (*fcc*) Fe lattice has been performed using the DFT PAW (Density Functional Theory Projector Augmented Wave) method as implemented in the VASP computer code. Within the framework of this study, the calculations of single vacancy, O, and Y impurities have been performed. Pair-wise interactions between vacancy, O, and Y have been calculated along with the assessment of the binding energies between these defects. The interactions between multiple defects have also been calculated. Migration barriers have been assessed using the NEB (Nudge Elastic Band) method. Due to an initial presence of low-concentration Ti impurities in steels, which can form both TiO and YTiO precipitates, additional first principles calculations on the corresponding models have been carried out as well. The results of performed calculations reveal the major factors contributing in the formation of the ODS steels.

Keywords: oxide dispersed strengthened steels (ODS), *ab initio* calculations, density functional theory

1 Introduction

Oxide dispersed strengthened (ODS) steels are considered as the promising structural materials for future fusion reactors. The implementation of ODS steels allows increasing the operating temperature of the reactor by 100°C, which noticeably improves its efficiency. Both size and spatial distribution of the yttrium oxide particles, which can include, *e.g.*, Ti atoms naturally distributed in steels, affect the mechanical properties of the ODS steels and their radiation resistance. However, the mechanisms of oxide particle formation in ODS steels are not fully understood yet.

Small amounts of Ti are added during the mechanical alloying of yttria allowing to refine the dispersion of the reinforcing oxides during hot isostatic pressing (HIPping). As the size of Ti atom is very similar to the size of Fe atom, the former is substituting regular iron atoms in the Fe lattice much easier compared to yttrium substitute atoms, while oxygen atoms may both substitute regular iron atoms in the Fe lattice and occupy interstitial positions.

ODS steels are manufactured during the mechanical alloying followed by the HIP process at temperatures of around 1000-1200 K under the pressure of 100 MPa. ODS particles found after HIPping are the remnants of initial oxide powder that are formed during MA. This may be supported by the fact that the HIPping temperatures are lower than yttria melting temperature so thermal process does not occur during the oxide particle transformation. There are experimental evidences that after milling a noticeable part of Y and O atoms can be decomposed from

yttria clusters in steel matrix with concentrations above their equilibrium solubility. In this case, the precipitation of Y₂O₃ nanoparticles can occur already at the HIPping stage as a result of yttrium-oxygen co-precipitation.

2 Computational details

VASP 5.2 computer code based on the Density Functional Theory (DFT) approach with a plane-wave (PW) basis set combined with the Perdew-Wang-91 GGA (Generalized Gradient Approximation) non-local exchange-correlation functional has been used to perform *ab initio* calculations [1]. The core electrons are described using the Projector-Augmented Wave method (PAW). Its computational procedure includes an iterative solution of Kohn-Sham equations, which is based on residuum-minimization and optimized charge-density mixing routines, it employs a plane-wave (PW) basis set combined with the PAW scalar relativistic pseudopotentials [2]. The latter include Fe core electrons of (4s¹3d⁷ outer shell), O (2s²2p⁴), Y (4s²4p⁶5s¹4d²), and Ti (3p⁶4s²3d⁴) atoms with 8, 6, 11, and 12 external electrons, respectively.

To define the calculation parameters necessary to obtain plausible results numerous preliminary test calculations have been performed. Some basic lattice parameters such as lattice constant, bulk modulus, cohesive energy, and vacancy formation energy assessed basing on these calculations have been found to be in a good qualitative agreement with the ones reported in the experiments and other theoretical studies.

The cut-off kinetic energies should be set to at least 800 eV, the k-point sets in the Brillouin zone should be at least $7 \times 7 \times 7$ k -mesh for supercells (SCs). The supercell models used in the calculations are cubic, with the extension of $4a_0 \times 4a_0 \times 4a_0$ containing 64 atoms, respectively, while the calculated optimized lattice constant has been found to be 3.448 Å [3-6].

3 Results and Conclusions

The results of the calculations prove that vacancies play a crucial role in the formation of the ODS nanoparticles in ODS steels as they play essential role in migration of impurity atoms inside *fcc*-Fe lattice (oxygen, titanium and yttrium) and stabilize defect complexes.

The smallest binding energies in the configurations when O atoms occupy the substitute positions have been

Gopejenko A, Zhukovskii Y F, Mastrikov Y A,
Kotomin E A, Piskunov S, Vladimirov P V

found when two Y or two Ti atoms as well as Y and Ti atoms are positioned as the 1NN. The binding energies between the defects very moderately increase with the growth of the distance between two Y or Ti atoms in Y-O_{Fe}-Y or Ti-O_{Fe}-Ti configurations as well as Y and Ti atoms in Y-O_{Fe}-Ti configurations when two Y or Ti atoms as well as Y and Ti atoms are 2NN, respectively.

A pattern between the binding energies and the displacements of the defect atoms is established: the larger of the displacement of the defect atoms towards each other during the relaxation, the larger is their binding energy.

The distance between the defect atoms has decreased more in the calculated Y_{Fe}-O_{Fe}-Ti_{Fe} compared with Y_{Fe}-O_{Fe}-Y_{Fe} configurations, which means that the local expansion of the crystalline lattice caused by the induced defects is lower. This might explain the smaller average size of YTiO particles comparing with Y₂O₃ particles.

References

- [1] Kresse G, Furthmüller J 2012 *VASP the Guide (Release 5.2.12)* University of Vienna
- [2] Kresse G, Joubert D 1999 *Phys Rev B* **59** 1758-75
- [3] Gopejenko A, Zhukovskii Yu F, Vladimirov P V, Kotomin E A, Möslang A 2010 *J Nucl Mater* **406** 345-50
- [4] Gopejenko A, Zhukovskii Yu F, Vladimirov P V, Kotomin E A, Möslang A 2011 *J Nucl Mater* **416** 40-4
- [5] Gopejenko A, Zhukovskii Yu F, Vladimirov P V, Kotomin E A, Möslang A 2012 *Proc. NATO ARW „Nanodevices and Nanomaterials for Ecological Security” (Eds. Shunin Yu N and Kiv A E, Springer: Dordrecht, 2012)* 149-60
- [6] Gopejenko A, Zhukovskii Yu F, Kotomin E A, Mastrikov Yu A, Vladimirov P V, Borodin V A, Möslang A 2016 *Phys Status Solidi B* **253** 2136-43