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Thesis: First principles simulations on yttrium and oxygen precipitation inside fcc-Fe lattice

Abstract:

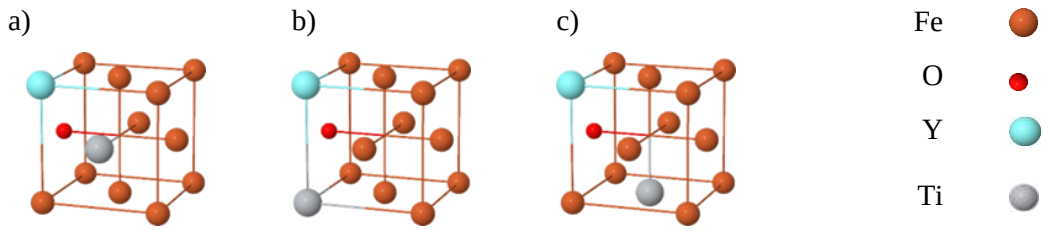
The oxide dispersed strengthened (ODS) steels are considered as the promising structural materials for future fusion reactors. The implementation of ODS steels allows increasing the operating temperature of the reactor by 100°C, which noticeably improves its efficiency. Both size and spatial distribution 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.

The presented PhD Thesis is the first systematized first principles description of interactomic interactions in ODS nanoclusters synthesized in *fcc*-Fe. The chosen approach for the *ab initio* calculations performed on *fcc* Fe lattice has been tested on basic parameters such as lattice constant, bulk modulus cohesive energy as well as on V_{Fe} vacancy formation energy. The results of the calculations are in a good agreement with both experimental data as well as with other theoretical studies. This means that the methods used in this work allow getting the plausible results.

DFT PAW method has been used to perform large-scale calculations on the basic properties of bulk *fcc*-Fe lattice and the effects of single vacancy, O, Ti and Y impurities on those properties. Such properties of the bulk *fcc*-Fe lattice as lattice constant, bulk modulus, and cohesive energy have been calculated being in a good qualitative agreement. The formation energies of the single defects as well as the vacancy formation energy have been assessed. The latter is in a good agreement with other simulations. It has been found that the supercell with the extension of 4×4×4, the cut-off energy of 800eV, and the *k*-point mesh of 7×7×7 are required to achieve the plausible results.

The modeling of the *pair-wise* dopant interactions in *fcc*-Fe lattice has been performed for Y_{Fe}–Y_{Fe}, Y_{Fe}–V_{Fe}, Y_{Fe}–O_{Fe}, Y_{Fe}–O_{oct}, Ti_{Fe}–Ti_{Fe}, Ti_{Fe}–V_{Fe}, Ti_{Fe}–O_{Fe}, Ti_{Fe}–O_{oct}, O_{Fe}–O_{Fe}, V_{Fe}–V_{Fe}, and O–V_{Fe} defect pairs in *fcc*-Fe followed by the calculations of the more complex defect configurations such as the configurations with three and four V_{Fe}.

The large-scale calculations of atom-substituted *triple-wise* interactions between Y_{Fe}–O_{Fe}–Y_{Fe}, Y_{Fe}–O_{oct}–Y_{Fe}, Ti_{Fe}–O_{Fe}–Ti_{Fe}, Ti_{Fe}–O_{oct}–Ti_{Fe}, Y_{Fe}–O_{Fe}–Ti_{Fe} (Figure 1), Y_{Fe}–O_{oct}–Ti_{Fe} atomic configurations of precipitates have been performed as well, however, without inclusion of V_{Fe} vacancies.



Figures 1. Model of Y_{Fe} and Ti_{Fe} atoms as 1NN (a), 2NN (b) and 3NN (c) neighbours, while O_{Fe} as the 1NN to both Y_{Fe} and Ti_{Fe} atoms.

The migration energies and trajectories of Y atom (possessing the largest diameter among atoms considered in this study) inside pure and doped *fcc*-Fe lattice have been calculated using the Nudge Elastic Band (NEB) method as it provides the most accurate results for the migration trajectories.

The results described in this PhD Thesis is a major step towards the modeling of the yttrium oxide particle precipitation required to understand deeper the mechanisms of ODS steels formation.

The results of the calculations have been systematized and uploaded to our partners in IAM-AWP (KIT), Karlsruhe to form a database of the interactions between the defects in iron lattice, which should allow using these results as the base for further ab initio as well as for Lattice Kinetic Monte-Carlo modelling of the ODS steel formation.