# *Ab initio* calculations of Ti pair-wise interactions inside *fcc*-Fe lattice

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**Abstract**

Addition of the metallic Ti species in the $Y_2O_3$ powder before mechanical alloying leads to the formation of $Y_2Ti_2O_7$ particles in ODS steels. In this case the average size of the ODS particles achieves up to 5nm, which is smaller than the size of $Y_2O_3$ ODS particles (10-20 nm). This results in the interest to study the interaction between two Ti atoms, Ti and vacancy as well as between Y and Ti in *fcc* Fe lattice. As the size of the Ti atom is very close to the size of Fe atom, the former can only substitute regular atoms in the Fe lattice, similarly to Y impurity atoms.

*Keywords:* ODS steels, density functional theory, ab initio calculations

## 1 Introduction

Reduced activation steels strengthened by yttria precipitates are promising structural materials for future fusion- and advanced fission-reactors. They show very promising resistance to radiation-induced creep and swelling, two of the main mechanisms of materials degradation. Both size and spatial distributions of oxide precipitates significantly affect mechanical properties and radiation resistance of ODS steels. The mechanisms of ODS nanoparticle formation as well as their stability under irradiation are still not well understood. Both experiments and simulations indicate that extended mechanical alloying leads to the dissolution of $Y_2O_3$ particles in the steel matrix during the mechanical alloying. Yttrium and oxygen dissolved above equilibrium solubility limits seem to precipitate during consolidation of mechanically alloyed powder. The processes involved in the particle nucleation are very difficult to study experimentally but they can be simulated using advanced techniques of multiscale modeling. Since titanium can exist as natural impurity in ODS steels its presence in iron lattice does not result in the marked reconstruction of the latter. On the other hand, Ti stabilizes yttria precipitates in ODS steels due to its higher affinity towards oxygen as compared to Y.

## 2 General

The first principles calculations have been performed using the *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 non-local exchange-correlation functional for $\gamma$-Fe. The core electrons are described using the Projector-Augmented Wave method (PAW). These pseudopotentials include Fe core electrons of ($4s^1 3d^7$ outer shell), O ($2s^2 2p^4$), Y ($4s^2 4p^6 5s^1 4d^2$), and Ti ($3p^6 4s^2 3d^4$) atoms with 8, 6, 11, and 12 external electrons, respectively.

To identify the calculation parameters required to obtain plausible results, numerous preliminary calculations have been performed and the results of these calculations have been compared with the ones reported in experiments and other theoretical studies. These calculations have shown that to achieve reliable results, 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 7×7×7 *k*-mesh for supercells (SCs) [1]. Our model supercells are cubic, with the dimensions of $4a_0 \times 4a_0 \times 4a_0$ and $5a_0 \times 5a_0 \times 5a_0$, extensions (containing 64 and 125 atoms, respectively), the calculated optimized lattice constants of which have been found to be 3.448 Å.

## 3 Conclusion

The interactions between two titanium atoms as well as between Ti atom and a vacancy are qualitatively similar to the interactions between two Y atoms and between Y atom and a vacancy. However, the absolute values of the calculated binding energies are smaller in the configurations containing Ti atoms. It has been found that the displacement of titanium atom in the direction of the vacancy in the configuration, where Ti atom and the vacancy are the first nearest neighbors, is 0.43 Å, which is smaller than the displacement of Y atom towards the vacancy (1.25 Å) in the similar configuration.

## References

[1] Gopejenko A, Zhukovskii Yu F, Kotomin E A, Mastrikov Yu A, Vladimirov P V, Borodin V A, Möslang A 2016 *Ab initio* modelling of Y–O cluster formation in *fcc*-Fe lattice *Phys. Status Solidi B* **253**, 2136-43