

## Influence of Dopants on Mechanical Properties of Steel: A Spin-Polarized Pseudopotential Study

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### Abstract

Density functional theory and pseudopotentials were used to study reaction of the ferrite grains interface (doped with C, P, N, Ti, Ti+N and Ti+C) on deformations. It was shown that impurities could increase or decrease the tensile strength and the elongation limit. The best effect was demonstrated for cases when Ti presents simultaneous with C; the worst case is doping iron with P. As for the shift modulus, effect is not significant.

**Keywords:** Ab initio simulation;  $\alpha$ -Fe; Tensile strength; Shift modulus; Dopants influence

### Introduction

Low carbonized steel is a well-known Fe alloy used as a material for various engineering details and constructions. Usually it contains up to 0.2 per cent of carbon and some small amounts of other dopants. There are some works where influence of dopants on the mechanical properties of steel is studied on the atomic level [1-5]. However, in the most of them only some energetic characteristics are studied, while engineers are interested in technical parameters. Here we present results of the tensile strength and the shift modulus calculations for the doped Fe.

### Methods and Models

As real steel is a polycrystalline material consisted mainly of  $\alpha$ -Fe grains, its durability depends mainly on the durability of grain interfaces (borders). For this reason our investigation is limited with studying of the interface between two grains of  $\alpha$ -Fe.

It is well known that  $\alpha$ -Fe is a ferromagnetic with magnetic polarization of  $2.2 \mu_B$  per atom, bcc-lattice with period  $a=2.867 \text{ \AA}$ , and cohesion energy of 5.48 eV. In this work we used the spin-polarized version of DFT realized within the FHI96md package [6] based on the density functional theory (DFT) [7,8] and the pseudo-potential method [9]. This package was previously used with advantage for many systems, including transition metal compositions [10-14]. In all cases, the generalized gradient approximation [15] to description of the exchange-correlation interactions has been chosen and the optimization of the atomic geometry has been performed. All pseudopotentials were constructed with the FHI98PP package [16]. They were checked for the absence of the so-called 'ghost' states and were used for founding the equilibrium lattice parameters, magnetic and the cohesion energy of  $\alpha$ -Fe.

To model the bulk bcc  $\alpha$ -Fe we used a cubic cell with two iron atoms: one atom was placed in the lattice cell corner; the second atom was situated in the center of the cell. The energy cut-off for the plane wave set was equal to 40 Ry and the special k-point (0.25; 0.25; 0.25) was used. The self-consistency convergence was provided by stabilizing the total energy with an accuracy of 0.005 eV per atom. We have found the equilibrium lattice constant of 2.88  $\text{\AA}$ , magnetic moment of 2.0  $\mu_B$ , and cohesion energy of 4.5 eV, in satisfactory accordance with experimental data.

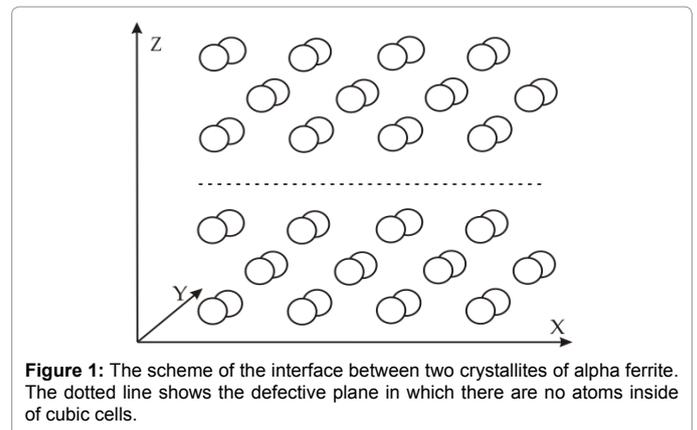
An interface between two  $\alpha$ -Fe grains was modeled as a contact

of two thin crystalline slabs having infinity dimensions in X and Y directions. Thickness of the each slab was made of three atomic layers. The interacting slabs approached among themselves before the minimum of their total energy was achieved. The scheme of such system is given in Figure 1.

In order to test our approach we calculated the interface energy (the energy gain of iron grains bonding) and have obtained the value of 1.33 J/m<sup>2</sup>. According to refs. [5,17] published values of the grain interface energy of Fe lie in the interval of 0.47-1.63 J/m<sup>2</sup>.

After leading of the system in a state with the minimum energy we made computer experiments of two types (Figure 2). The top panel: investigation of the reaction of the interface to break; the down panel: investigation of the reaction of the interface to shift.

In the stretch case we found the variations of the total energy  $\Delta E$  as functions of elongation  $\Delta Z$ , and then the applied strength P was



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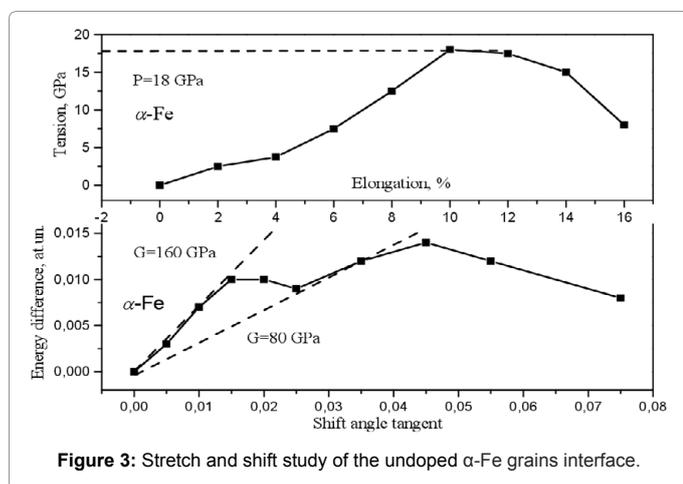
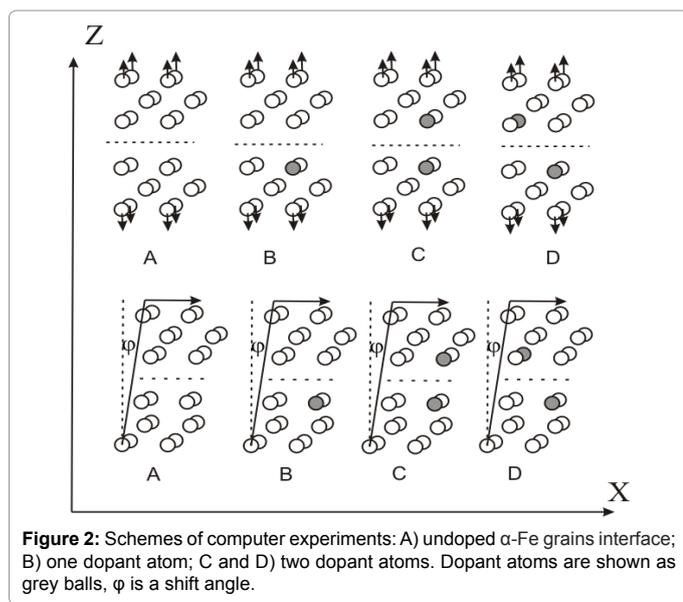
calculated according the formulae  $P = \frac{\Delta E}{\Delta Z} \frac{1}{S_{XY}}$ , where  $S_{XY}$  is the system square in the XY plane. In the shift case we studied the dependence of  $\Delta E$  on  $\text{tg}\phi$ , where  $\phi$  is the shift angle, and calculated the shift module  $G = \frac{\Delta E}{\Delta X} \frac{1}{S_{XY}} \frac{1}{\text{tg}\phi}$ .

## Results and Discussion

### Undoped $\alpha$ -Fe

First of all we studied reaction of the undoped iron system on stretching along Z direction and on shift along X direction. Atoms of upper and down planes were moved step-by-step and fixed at the each step. Other atoms were able to relax up and to find equilibrium positions. The dependences of tension on elongation and energy on tangent of the shift angle are presented in Figure 3.

The top panel of this figure demonstrates the strength limit of 18 GPa for breaking the undoped  $\alpha$ -Fe grains interface. The down panel shows that the shift process has two stages. Firstly, the total energy grows sharply with the shift modulus of 160 GPa; secondly, the shift modulus decreased to 80 GPa. Comparatively, experimental value of



tensile strength is 60 MPa for the low carbonized steel and 1.3 GPa for single-crystalline whiskers. The published shift module value is 14 GPa [3].

### Dopants influence

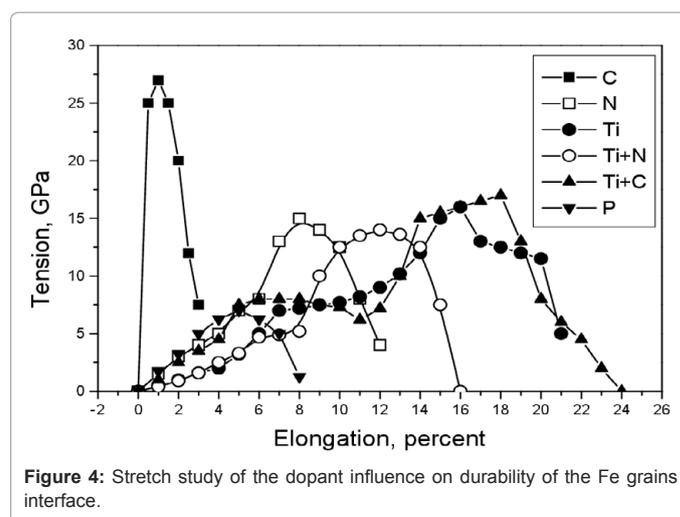
We placed dopant atoms as it is shown in Figure 2B-2D. Namely, for single-atomic cases we replaced one atom of the interface with C, P, N or Ti atom. For two-atomic cases (TiN or TiC) dopant atoms were placed on both sides of the interface. Results of calculations are presented in Figure 4 and Table 1.

It is clear (Figure 4) that presence of carbon increases the tensile strength by 1.5 times in comparison with undoped ferrite; N and Ti+N decrease it approximately by 20 percent. The Ti and Ti+C cases demonstrate the tensile strength very close to the case of undoped iron. At another hand addition of carbon reduces the limit of elongation to 1 percent (for undoped  $\alpha$ -Fe it is 10 percent); nitrogen reduces it to 8 percent; while Ti, Ti+N and Ti+C increase its value up to 14-18 percent. As for phosphorus it decreases strongly both the tensile strength and the limit of elongation. In more details results are collected in Table 1.

Influence of dopants on the shift behavior of the Fe grains interface is much less significant than their effect for the stretch characteristics. Our modeling shows that in all doped cases the dependence of the shift module on the shift angle tangent looks like that of the undoped Fe case, and its value varies between 70 and 170 GPa.

### Conclusion

Quantum-mechanics modeling of the  $\alpha$ -Fe grains interface as a contact of two nano thin slabs lets us to obtain adequate data of dopants influence (C, P, N, Ti, Ti+C and Ti+N) on mechanical properties of steel. Summarize all results we can conclude that addition of Ti (single or with C) increases significantly the elongation limit keeping approximately the level of the tensile strength of un-doped iron. Thus, addition of Ti in the C doped  $\alpha$ -Fe can improve elasticity of steel details and constructions at low temperatures. Phosphorus is the worst impurity in steel.



System	Undoped Fe	Fe+C	Fe+N	Fe+Ti	Fe+Ti+C	Fe+Ti+N	Fe+P
P, GPa	18	27	14.8	15.5	16.5	14.5	7.1
L, percent	10	1	8	16	18	12	5

Table 1: Tensile strength  $P$  and elongation limit  $L$  for the Fe grains interface.

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