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Ab initio formation energies of Fe–Cr alloys

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Abstract

We have calculated ab initio lattice parameters, formation energies, bulk moduli and magnetic moments of Fe–Cr alloys. The results agree well with available experimental data. In addition to body centered cubic (bcc) alloys, which are representative of ferritic steels used in fast neutron reactors, face centered cubic (fcc) and hexagonal close packed (hcp) phases were considered in order to complete a theoretical database of thermodynamic properties. Calculations were done for the ferromagnetic phase, as well as for a phase with local moment disorder, simulating the magnetic structure at high temperatures. For the latter case, the formation energy of the alloy is strictly positive smooth function of chromium concentration, in agreement with experiments performed at high temperature. In the ferromagnetic case, a negative mixing enthalpy is found for chromium concentrations below 6%. Our observation is consistent with the experimentally observed inversion of the ordering trend, as well as with formation of the chromium rich α' phase at Cr-concentrations above 9%, occurring at $T < 900$ K.

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1. Introduction

The use of ferritic martensitic steels as structural material for fast neutron reactors has been advocated due to their relatively low rate of swelling at elevated temperatures [1–3]. A significant body of experimental results have been accumulated and swelling rates in ion/electron irradiated steels have been satisfactorily explained by the dislocation bias mechanism. However, theoretical understanding of the mechanisms responsible for swelling of neutron irradiated steels, i.e. under cascade conditions, remain on a qualitative level [4–6].

In order to quantify the analysis, multi-scale modeling is required. The numerical tools that are applied include ab initio solutions to the Schrödinger equation, fitting of effective many-body interaction potentials, molecular dynamics simulation of recoil cascades, Monte Carlo simulation of defect evolution and quasi-continuum rate theory.

Atomistic simulations depend strongly on the validity of the effective interaction potential adopted. For pure iron, several many-body potentials have been developed [7–9]. For Fe–Cr, the only potential found in literature applied the experimental formation energies of Fe–Cr in the fitting procedure [10]. However, the measurements were made for paramagnetic alloys at a temperature of 1600 K [11,12]. Therefore, it is not obvious if this potential is able to reproduce the inversion of a tendency to form an ordered compound to a tendency towards the phase separation observed in bcc Fe–Cr alloys for Cr concentrations above 9% at $T < 750$–900 K [13–15]. The formation energy and other thermodynamic properties of monocrystalline Fe–Cr in the ferromagnetic phase is difficult to measure, and hence one has to rely on

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theoretical approaches. It is the purpose of the present paper to provide such data for use in the development of a many-body potential for Fe–Cr. In what follows, we will describe first principle calculations of thermodynamic and magnetic properties. Special attention is devoted to Cr concentrations below 15%, being of relevance for materials actually used in reactors.

We start by briefly describing the theory behind the implemented computational technique. Specific details of the calculations are highlighted. Results are presented for lattice parameters, magnetic moments, formation energies and bulk moduli for bcc alloys. The stability of bcc and hcp crystal structures relative to fcc is calculated. Comparison with available experimental data is made. Finally we discuss interesting features that we find in the formation energy of ferromagnetic bcc alloys as function of Cr content.

2. Density functional calculations

2.1. Theory

In ab initio calculations of energies and structural and magnetic properties of random Fe–Cr alloys, the Schrödinger equation cannot simply be solved for the complete many-body system. Rather, some kind of approximation technique has to be used. We carry out calculations in the framework of the *density functional theory* (DFT) [16]. It allows us to solve the so-called Kohn–Sham equations. Within this scheme, the Schrödinger equation is formulated for an effective one-electron potential, decreasing the complexity of the problem enormously. The self-consistent one-electron potential and the electron density are obtained within the *local density approximation* (LDA) [17]. Using the LDA charge density, the total energy may be calculated either from the LDA energy functional, or from the *general gradient approximation* (GGA). The procedure was tested against calculations where the potential, density, and total energies were obtained self-consistently within the same functional. Results for the thermodynamic properties were found to be indistinguishable from those obtained within the scheme mentioned above. In this work we calculated GGA total energies, because it is well known that LDA predicts the wrong ground state for Fe.

Within our method, the one-electron wavefunction is expanded using a basis set of *exact muffin-tin orbitals* (EMTO) [18–20]. Moreover, the Kohn–Sham equations are solved using the so-called Green's function technique [21]. During the iterations towards the self-consistency, we use the *spherical cell approximation* (SCA) [21] with overlapping potential spheres that cover the space. The latter is much more numerically efficient as compared to solving the problem for the full non-spherically symmetric potential. However, the total energies are corrected for the said approximations by using the *full charge density* (FCD) method [22]. As has been mentioned above, with the FCD we calculate the energy using the GGA functional. The reliability of the combined technique is justified by the variational properties of the total energy functional. In practice, the accuracy of the method has been demonstrated in Ref. [22].

The problem of substitutional disorder in Fe–Cr systems is treated within the *coherent potential approximation* (CPA) [23–26] which is known to give reliable electronic structure and total energies for completely random alloys [27]. A comprehensive study of structural stability of non-magnetic bcc Fe–Cr alloys was carried out earlier within the CPA, in combination with the generalized perturbation method, by Turchi et al. [28]. In that work, magnetic moments on Fe and Cr were artificially suppressed, because the magnetism was supposed to have little effect on the resulting chemical order. At the same time, Akai and Dederichs [29], and Kulikov and Demangeat [30] investigated, within the CPA, magnetic properties of bcc Fe–Cr, while Ling et al. [31] studied the influence of magnetism on the short-range order in $Fe_{30}Cr_{70}$. In particular, Akai and Dederichs [29] have shown that the energy difference between the ferromagnetic alloys and the alloys where magnetic moments point out randomly 'up' or 'down' (the so-called disordered local moment model) is substantial, especially in alloys with low Cr concentration. The influence of magnetism on the structural stability in Fe–Cr alloys was also investigated by Moroni and Jarlborg [32] using the structural inversion method and the tetrahedron cluster expansion. They calculated mixing enthalpies of random ferromagnetic, as well as non-magnetic Fe–Cr alloys. Unfortunately, the authors of this work pointed out themselves that their results were not fully converged. Due to the long range of the effective cluster interactions in this system (also found in Ref. [28]) the tetrahedron cluster expansion is clearly not sufficient. Still, their results show that the magnetism may have a profound effect on the stability of Fe–Cr alloys. In the present study we pay particular attention to this problem.

2.2. Details of calculations

The calculations were performed with a basis set of s, p, d and f orbitals. The CPA works very well for the Fe–Cr alloys since the atoms are of similar sizes and atomic displacements from the ideal sites of the underlying lattice are extremely small [33]. Though the local lattice relaxations are believed to be quite important for understanding of the nucleation of the ordered σ phase in Fe–Cr [28], they may be safely neglected in the calculation of the thermodynamic properties of random alloys, which is the subject of the present paper. In terms of concentration, the calculations were taken at 5% intervals, except for the low-Cr region ($\leqslant$10% Cr) where the interval was 2%. An extra point at 3% Cr was added. Depending on the proximity to the non-monotonic behaviour (to be discussed below), the number of different atomic volumes considered at each concentration ranges from 6 to 26. The highest number of atomic volumes was naturally also in the low-Cr region.

For the FCD–EMTO–CPA calculations, 1240 points in the irreducible part of the Brillouin zone were used for bcc alloys, while 505 points were used for fcc and 503 points for hcp alloys. The calculations converged to the order of 10^{-6} Ry. The equilibrium values of thermodynamic properties were obtained by fitting the energy vs. volume data to different equations of state. In the cases where we discovered peculiarities we used a cubic spline fit. The regular cases were fitted using the analytical Morse-type equation of state [34].

For temperatures below 1000 K, the Fe-rich alloy is stable in a *ferromagnetic* (FM) bcc phase. Above the Curie temperature, the alloy is *paramagnetic* (PM) [12]. The latter situation is simulated by means of the so-called *disordered local moments* (DLM) model for the spin orientations [35]. Within the DLM picture, a paramagnetic binary $\mathrm{Fe}_c\mathrm{Cr}_{1\text{-}c}$ alloy is modeled by the random quaternary alloy $(\mathrm{Fe}\uparrow\text{–}\mathrm{Fe}\downarrow)_c(\mathrm{Cr}\uparrow\text{–}\mathrm{Cr}\downarrow)_{1\text{-}c}$, with equal amount of spin up (↑) and spin down (↓) atoms. Thus, though formally all our calculations are still performed at temperature 0 K the effect of the loss of net magnetic moment above the Curie temperature on the alloy total energy is captured within this scheme. Of course, such an approach does not include the magnetic entropy contribution to the free energy. But in the present study we calculate those thermodynamic properties, which are defined through the total energies, and for which an entropic contribution may be safely neglected. In any case, the use of the DLM model leads us to a picture that is much closer to the real situation in transition metal alloys above the Curie temperature, as compared to more conventional non-magnetic calculations, where magnetic moments on alloy components are suppressed artificially. Accordingly, for the fcc (γ-phase) and hcp Fe–Cr calculations we also use the DLM.

3. Results

Fig. 1 displays the calculated lattice parameter of random Fe–Cr alloys as a function of Fe concentration (here and in the following, concentrations are given in atomic percent) for three different crystal structures. As one can see the theoretical results for the ferromagnetic bcc alloys agree well with the experimental values. The concentration dependence in this case is quite weak, because the bcc Fe and Cr have similar lattice constants. On the other hand, we see stronger concentration dependences in the case of fcc and hcp alloys. Lattice parameters of fcc and hcp Fe, which within the DFT have a low spin magnetic ground state most probably with complicated magnetic configurations, are smaller as compared to the high spin ferromagnetic bcc Fe due to the magnetovolume effect [36–39]. On the contrary, the lattice parameter of bcc Cr is lower than those of fcc and hcp Cr because the bcc phase has much higher cohesive energy while the contribution to the total energy due to magnetism is very small [29]. Therefore, though there is no experimental information on the lattice parameters of fcc and hcp Fe–Cr alloys, the calculated values seem reasonable.

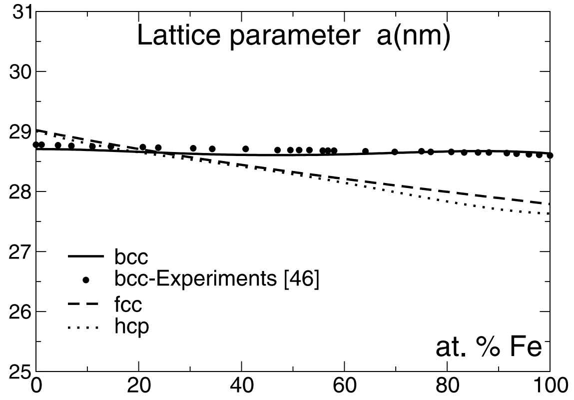

Fig. 1. Calculated lattice parameters a of random Fe–Cr alloys as a function of Fe concentration for three different close-packed structures, bcc (solid line), fcc (dashed line), and hcp with ideal c/a ratio (dotted line). The bcc data are shown for the ferromagnetic alloys. The results obtained within the disordered local moments are very close to the ferromagnetic results. The experimental data for bcc Fe–Cr alloys from Ref. [46] is shown by filled circles.

In Fig. 2, the magnetic moment of bcc Fe–Cr is presented. Again, we see a good agreement between experiment and theory for bcc alloys for Fe concentration above 30 at.%. For lower Fe concentration the experimental situation with magnetism becomes uncertain, while pure bcc Cr has a magnetic structure with transverse or longitudinal spin density waves, depending on the temperature [40]. We did not investigate this problem in details, because we are mainly interested in properties of bcc Fe-rich alloys. For the same reason we did not study complicated magnetic properties of fcc and hcp alloys. Note, that our calculated values for bcc Fe–Cr alloys also agree with other first-principles studies of magnetic properties in this system carried out within the CPA [29,30], or within alternative real space approaches [32,41].

Unfortunately, there are no experimental data for the formation energies of random Fe–Cr alloys in the temperature interval relevant to reactor operation

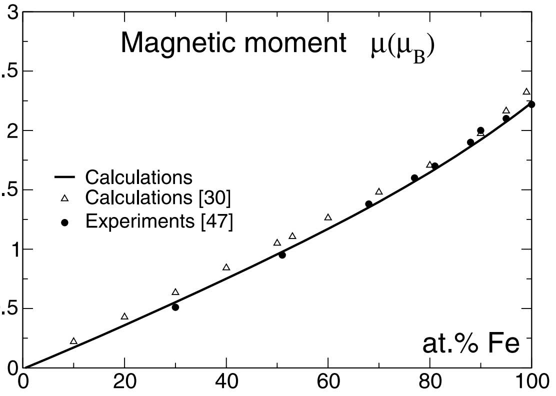

Fig. 2. Calculated magnetic moments μ (solid line) of random bcc Fe–Cr alloys (in Bohr magnetons μ_B) as a function of Fe concentration. The experimental values were taken from Ref. [47]. For comparison the results of CPA calculations for the same system from Ref. [30] are also shown with triangles.

(600–1000 K). The experimental data [11,12] were obtained at 1600 K, where the alloy is in a PM phase. Hence, the calculations presented in Fig. 3 were performed using the DLM model and with the bcc Fe and Cr (also in the DLM spin configuration) taken as standard states. The calculated values are in very good agreement with experiment and the slight overestimation is due to the neglect of the short-range order in our CPA calculations. The latter is present in Fe–Cr alloys [13,33] for which the experiments were conducted. In Fig. 3 we also show mixing energy for fcc Fe–Cr alloys. Note that as compared to the experiment, the calculated fcc energy underestimates the experimental values by approximately 4 kJ/mol, but that the angle of the curve is in very good agreement with the experiment. Here we would like to point out that the experimental values for the low Cr concentration were obtained by means of extrapolations [12], and therefore are probably not as reliable as values obtained in direct measurements.

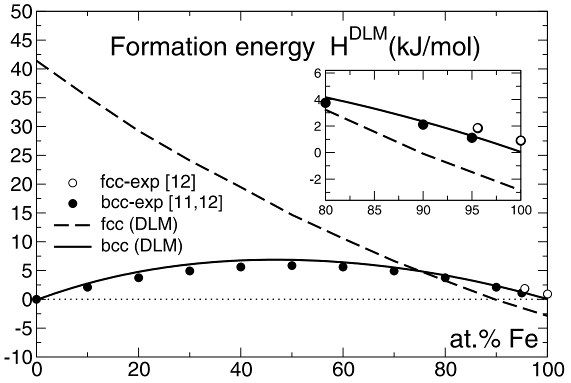

Fig. 3. Calculated mixing enthalpy (H^{DLM}) of random Fe–Cr alloys obtained within the DLM model as a function of Fe concentration. The standard states (bcc Fe and bcc Cr) were also calculated within the DLM model. Solid line shows the mixing enthalpy of bcc alloys, dashed line shows that of the fcc alloys. The experimental values for bcc (filled circles) and fcc (open circles) alloys [11,12] were obtained at 1600 K where the system is paramagnetic. The comparison is made to verify the reliability of our theoretical calculations.

The curves in Fig. 4 represent the structural energy difference in random Fe–Cr alloys, with ferromagnetic alloys in the bcc structure taken as zero line. As we can see, the FM bcc alloys are more stable as compared to all other systems considered in the present study in the whole interval of concentrations. In agreement with Ref. [29], we obtain that the DLM bcc phase is nearly degenerate with the FM bcc phase at low Fe concentration, but it is substantially higher in energy for Fe-rich alloys. This agrees with high Curie temperature of the bcc Fe. Moreover, in the DLM case the bcc structure becomes less stable with respect to the fcc structure in the low-Cr region which is consistent with the phase transition above the Curie temperature [12]. However, the entropy must substantially contribute to this transition, because as a matter of fact the hcp alloys are energetically more stable than the fcc alloys in the upper part of the concentration range. We do not see the hcp phase at ambient pressure [12]. However, the bcc Fe transforms to the hcp phase upon compression, and the hcp Fe is indeed stable at high pressures. We would also like to point out that we did not allow for complicated non-collinear magnetic configurations in this study. In particular, such configurations are believed to describe the ground-state ($T = 0$ K) magnetic structure of pure fcc Fe [37,42,43]. Thus, the energy difference between the fcc and the bcc alloys, as well as possibly between the

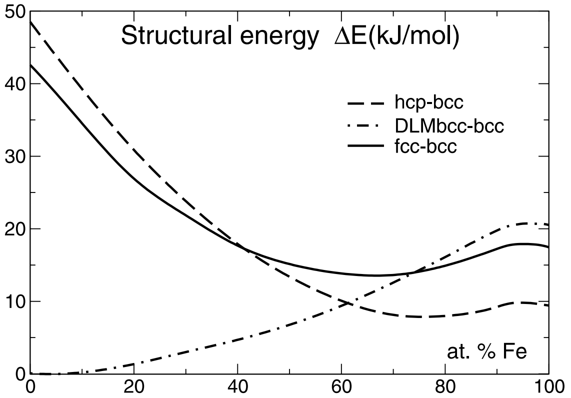

Fig. 4. Calculated structural energy difference ΔE between the different Fe–Cr structures (fcc, hcp and DLM bcc) compared to the ferromagnetic bcc alloy. The bcc is the zero line. The fcc is the solid line. The DLM bcc is the dash-dotted line and the hcp is the dashed line.

hcp and the bcc alloys, presented in Fig. 4 might be overestimated at $T = 0$ K. We still believe that the calculated results may be used as a source of information, e.g. for a fitting of the interatomic potentials, because at elevated temperatures any magnetic order in the fcc and hcp alloys should be destroyed, while it is present in the bcc phase. More complete analysis of the problem requires a consistent treatment of the spin dynamics and lattice vibrations, which is beyond the possibility of the current theory.

The formation energies of the ferromagnetic bcc Fe–Cr alloys presented in Fig. 5 are perhaps the most interesting results of the present study. Note, that here the ferromagnetic bcc Fe and bcc Cr are used as reference states. The lack of experimental data makes these calculations the unique source of information on the formation energy of random Fe–Cr. It is important to point out that in contrast to the paramagnetic case, the ferromagnetic alloys show substantial deviations from the regular solution behaviour. The most interesting part is the low-Cr region. As can be seen, the calculated formation energies are *negative* from 94% Fe to pure Fe, while they are positive for alloys with lower Fe concentration. It is impossible to conclude whether the random alloys are thermodynamically stable in the concentration interval above 94% Fe without a more complete study, which includes statistical mechanics simulations, as well as a consideration of intermediate intermetallic phases. But in any case, it is clear from the negative sign of the calculated formation energy that bcc Fe–Cr alloys must be relatively much more stable at low Cr concentrations. A possible reason for such a behaviour may be the so-called electron topological transition of the Fermi surface in this concentration interval [44].

The bulk modulus depends very sensitively on the energy–volume relation, since it is calculated from the second derivative of the energy with respect to the volume. Typically, calculations within DFT predict bulk moduli with accuracy 10–20%. Worth mentioning is also that the experimental values of the bulk modulus are usually obtained at room temperature and the calculations are done at 0 K. Speich et al. [45] has shown that the bulk modulus decreases by approximately 5% when going from near-absolute zero to room temperature, at least in isotropic materials. As can be seen in Fig. 6, the calculations overestimate the bulk modulus by roughly 15% for pure Fe. This is within the usual error of the DFT. At the same time, the error is up to 30% for pure Cr. As we have pointed out above, in the Cr-rich region the alloy has non-trivial magnetic properties. Hence the increasing error in theoretical values of bulk modulus towards higher Cr concentrations is to be expected.

For the same reason the results of fcc and hcp bulk moduli calculations are not included since they are somewhat dubious. They fluctuate rather strongly depending on changes in magnetic configurations and we are currently working on improving the stability of these calculations. At the same time, the bulk moduli for Fe-rich ferromagnetic bcc alloys are more reliable, because the magnetic configuration in this case is quite certain. The blow-up of the low-Cr region displays more closely the interesting behaviour taking place at these concentrations. Both the theory and the experiment show a peculiarity of the bulk moduli as a function of concentration. Note, that it occurs at the same composition where the formation energy deviates strongly from the regular solution model. The peculiarity on the concentration dependency of the bulk moduli has seemingly square-root shape which typically stems from an electron topological transition.

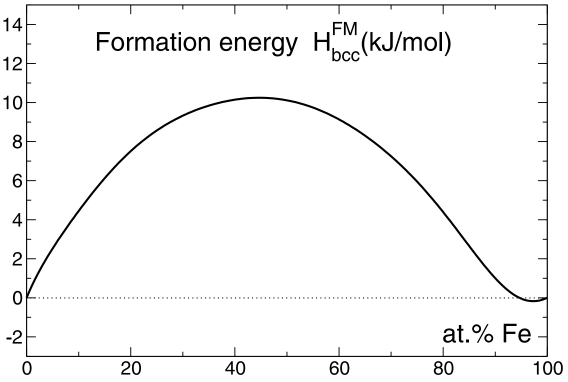

Fig. 5. Calculated mixing enthalpy (H^{FM}_{bcc}) for ferromagnetic bcc Fe–Cr alloys, corresponding to Fe–Cr in the low-temperature range ($T < 1000$ K).

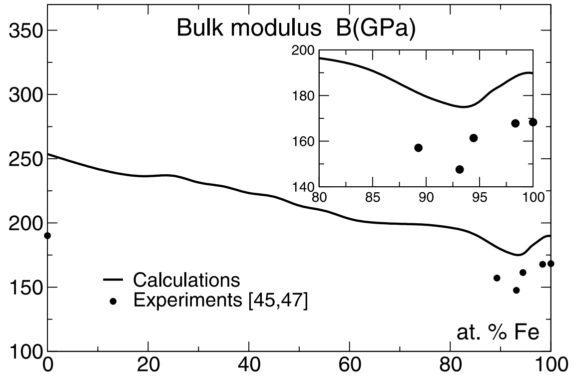

Fig. 6. Calculated bulk modulus B of ferromagnetic bcc Fe–Cr alloys (solid line) as a function of Fe concentration. The experimental data are shown with filled circles, and are taken from Ref. [47] for pure Fe and Cr and from Ref. [45] for a polycrystalline Fe-rich alloys. Insert in the figure emphasises the peculiarity of the bulk moduli which is present at low Cr concentrations.

4. Conclusion

The importance of this work consists mainly in the novel calculation of the formation energy and bulk moduli of random bcc Fe–Cr alloys in the ferromagnetic phase. This phase is relevant from technological point of view, while available experimental data [11] concern ordered alloys or the high temperature paramagnetic phase. We have found that the formation energy is negative for Cr concentrations below 6%. At the same time, it is positive for higher Cr concentrations, and it reaches a maximum of 10 kJ/mol for equimolar composition. Our observation is consistent with the experimentally known inversion of the short-range order in the system as a function of concentration [13], as well as with formation of the chromium rich α' phase at Cr-concentrations above 9%, occurring at $T < 900$ K [14,15]. Also, we observe that the bulk moduli, theoretical, as well as experimental, show a peculiarity around 6% Cr, i.e. in the same concentration interval where the mixing energy is negative. The most probable physical reason for these two effects is the electronic topological transition [44] taking place at this concentration. The peculiarities of the formation energy and the bulk moduli, underlined in our study, must be included in fitting of many-body interaction potentials aimed to study radiation damage in Fe–Cr steels by means of molecular dynamics simulations.

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