Ideal strength of ferromagnetic Fe-based alloys from first-principles theory

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(Dated: May 11, 2014)

The all-electron exact muffin-tin orbitals method in combination with the coherent-potential approximation has been employed to investigate the ideal tensile strengths of bcc ferromagnetic Fe and Fe1−xMx (M = Cr, Ni, Al, Co, Mn, and V) random alloys in the [001] direction. The present ideal strength is calculated to be 11.0 GPa for pure bcc Fe, in good agreement with the available theoretical data. For the Fe-based alloys, we predict that Co, Cr and V increase the ideal tensile strength, while Ni and Al decrease it. Manganese yields a non-monotonous alloying behavior. We show that the limited use of the previously established ideal tensile strengths model based on structural energy differences in the case of Fe-bases alloys is attributed to the effect of magnetism.

I. INTRODUCTION

The mechanical strength of real materials is usually controlled by the occurrence of grain boundaries, cracks, dislocations and other micro-structural defects. If such defects were not present, the strength would be limited by the stress at which the lattice itself becomes unstable with respect to a homogeneous strain. This stress referred to as the ideal strength or ideal tensile strength (ITS) is an upper bound strength of an ideal single crystal. The ideal strength is an inherent property of a defect-free material and can offer insight into the correlation between the intrinsic chemical bonding and the crystal symmetry, and has been accepted as an essential mechanical parameter of single crystal materials.1 The experimental data on the ideal strength are rather limited. The few available values were obtained from tensile tests for whiskers2,3 and from nanoindentation experiments.4

In recent years, considerable attention was paid to the computation of the ITS of elements or ordered alloys by first-principle methods. The ideal strength of refractory metals (such as Mo, Nb, V, and W), noble transition metals (such as Cu, Pt and Au), elements crystallizing in the diamond structure (Si, Ge, and C) as well as few ordered alloys (TiAl and Ni3Al) was extensively investigated.5–17 Among the body-centered cubic (bcc) metals, Fe received a great scientific interest.1,17–21 It was reported that, the [001] direction of Fe is the weakest direction in response to an uniaxial stress. It has been shown, that a bifurcation from the primary tetragonal deformation path (the Bain path) to a secondary orthorhombic deformation path occurs after the ITS on the primary path is reached.1 Thus, bcc Fe strained along the [001] direction fails by cleavage and not by shear as opposed to bcc V and Nb.12 In spite of all these theoretical efforts, the first-principles description of the ITS in substitutionally disordered alloys is rather limited. Li et al.22 investigated the composition dependent ITS of bcc vanadium-based nonmagnetic (NM) random solid solutions alloyed with chromium and titanium in various crystallographic directions employing the coherent potential approximation (CPA). To the best of our knowledge, no experimental or theoretical study has focused on the alloying effect on the ITS of Fe-based alloys. It is the purpose of this paper to bring forward a comprehensive study of the ideal strength to bcc ferromagnetic (FM) Fe-based random alloys.

Iron alloys are the most widely used engineering materials due to their excellent mechanical properties. For example ferritic Fe-Cr-based stainless steels have been considered as the primary structural materials in the first wall and blanket structure of future fusion reactor.23,24 Alloying plays a central role in designing advanced engineering materials with desired properties. Different solute atoms produce different effects on fundamental mechanical properties. Previous works focused on the effects of various typical solute atoms on the mechanical properties of Fe in the small deformation region, where the stress-strain relations are linear.25–30 However, the ideal strength describes the mechanical properties of the material beyond the elastic region.

In this work, using the exact muffin-tin orbitals method, we study the composition dependence of the ITS of FM Fe1−xMx alloys for various alloying elements, M = Cr, Ni, Al, Co, Mn, and V. The primary purpose of our work is to give an account of the application of the alloy theory to the ITS of bcc FM random alloys. Second, we aim to provide a consistent theoretical guide
II. COMPUTATIONAL METHOD

A. Total energy calculation

The first-principle method used in this work is based on density functional theory (DFT).\textsuperscript{31} We adopted the generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof (PBE)\textsuperscript{32} functional to describe the exchange-correlation interaction, which is well known to give the correct FM bcc ground state for Fe. The Kohn-Sham equations were solved using the EMTO method.\textsuperscript{33–35} The problem of disorder was treated within the CPA and the total energy is computed via the full charge-density technique.\textsuperscript{36–39}

The EMTO method is an improved screened Korringa-Kohn-Rostoker (KKR) method,\textsuperscript{33} where the full potential is represented by overlapping muffin-tin potential spheres. Inside these spheres, the potential is spherically symmetric and constant in between. By using overlapping spheres, one describes more accurately the exact crystal potential compared to conventional muffin-tin methods. Further details about the EMTO method and its self-consistent implementation can be found in previous works.\textsuperscript{33–35,38,39} The accuracy of the EMTO method for the equation of state, elastic properties, and the ideal strength in tension of metals and alloys has been demonstrated in a number of previous works.\textsuperscript{22,34,37,40–45}

The paramagnetic state of the Fe-based alloys was simulated by the so-called ordered localized moment (DLM) model.\textsuperscript{18–40} Within the DLM picture, the paramagnetic Fe and Fe\textsubscript{1−}M\textsubscript{x} binary alloys were described as a binary alloy Fe\textsuperscript{↑}Fe\textsuperscript{↓} and a quaternary (Fe\textsuperscript{↑}Fe\textsuperscript{↓})\textsubscript{1−}M\textsuperscript{↑}M\textsuperscript{↓}\textsubscript{x} alloy, with an equal amount of spin-up (↑) and spin-down (↓) components, respectively.

B. Ideal tensile strength calculations for bcc crystals

The principles of the response of bcc crystals to uniaxial loading were developed in a series of works by Milstein \textit{et al.}\textsuperscript{47–49} In this work, we computed the ITS in the [001] direction of bcc Fe and Fe-based alloys. Since [001] was already identified to be the weakest direction of bcc Fe,\textsuperscript{18,19,21} here we concentrated on this direction only. Assuming an uniaxial tensile load, the tensile stress \(\sigma(\varepsilon)\) can be calculated by\textsuperscript{15}

\[
\sigma(\varepsilon) = \frac{1}{\Omega(\varepsilon)} \frac{\partial E}{\partial \varepsilon},
\]

where \(E\) is the total energy per atom and \(\Omega(\varepsilon)\) is the volume per atom at a given tensile strain, \(\varepsilon\). The first maximum on the stress-strain curve defines the ITS, \(\sigma_m\), for the selected deformation path with corresponding maximum strain, \(\varepsilon_m\).

Uniaxial loading along the [001] direction reduces the symmetry of the bcc lattice to the body-centered tetragonal (bct) one on the primary deformation path. Clatterbuck \textit{et al.}\textsuperscript{1} reported a bifurcation from the primary deformation path to a secondary orthorhombic (orth) deformation path in Fe, however, the branching occurs for strains well above \(\varepsilon_m\). Thus, an isotropic Poisson contraction along the Bain transformation path describes appropriately the symmetry of the distorted Fe lattice up to \(\varepsilon_m\). The ideal tensile strength of the present Fe-alloys may nevertheless be influenced if this branching point shifts towards strains smaller than the maximum strain along the primary deformation path. We account for this possibility in this work.

On the primary tetragonal deformation path, the uniaxial strain energy,\textsuperscript{22} \(\Delta E(c; [001])\), describes the total energy change upon deforming the bcc crystal in the [001] direction, and relaxing it with respect to the dimensions in the (001) plane,

\[
\Delta E(c; [001]) = \min_a E(a, c) - E_0,
\]

here \(a\) and \(c\) denote the lattice constants of the quadratic basal plane and the height of the bct unit cell, respectively. The initial undistorted state corresponds to the equilibrium bcc structure with energy \(E_0\) and \(c = a\). At \(c/a = \sqrt{2}\), the bct lattice coincides with the face-centered cubic (fcc) lattice. On the secondary orthorhombic deformation path, we consider \(\Delta E(a_{\text{orth}}, b_{\text{orth}}; [001])\) and minimize the total energy with respect to the lattice parameters of the face-centered orthorhombic lattice, \(a_{\text{orth}}\) and \(b_{\text{orth}}\) (to describe the bifurcation from the primary tetragonal to the secondary orthorhombic strain path, the face centered tetragonal reference frame of the Bain transformation is used\textsuperscript{22}).

For a more detailed technical description of ideal strength simulations with EMTO, we also refer the reader to Ref. 22.

III. RESULTS

A. Ideal strength of bcc iron

To assess the reliability of our computational approach, we first performed the simulation of a tensile test in FM bcc Fe for uniaxial loading along the [001] direction. The theoretical equilibrium lattice parameter of bcc Fe
is 2.829 Å from our calculation, which agrees well with a full-potential value of 2.830 Å.\textsuperscript{50} The experimental lattice parameter, 2.868 Å,\textsuperscript{51} is 1.4% larger than the theoretical equilibrium value. The calculated spin magnetic moment of FM bcc Fe is 2.27 μB, which is approximately 2% larger than the measured value 2.22 μB.\textsuperscript{52} This overestimation of the magnetic moment of Fe is due to the employed GGA functional.

The magnetic order of the strained Fe lattice may change along the uniaxial loading process. For strains up to the branching point governed by the Bain transformation as discussed in the previous section. At zero strain, the ground state magnetic order is FM (bcc phase). The fcc state of Fe lying on the Bain transformation path (albeit at strains much larger than ε_m) exhibits a non-collinear spin arrangement as measured in fcc Fe precipitates and in thin fcc Fe films.\textsuperscript{53–55} That indicates that the ground state magnetic order of the strained bct Fe lattice begins to differ from FM order at some particular strain in the range between bcc and fcc along the primary transformation path. If this would be the case for ε ≤ ε_m, then additional magnetic order should be considered. However, there are strong indications that the FM order is the prevailing magnetic state for strains smaller than and somewhat above ε_m.\textsuperscript{20,56,57}

Clatterbuck et al.\textsuperscript{20} computed the ideal strength of Fe in the [001] direction considering the FM order, a collinear anti-ferromagnetic structure (AFM, magnetic moment sequence ↑↓↓) and a collinear double layer anti-ferromagnetic structure (DAFM, magnetic moment sequence ↑↑↓↓). Their results show that Fe remains FM up to the point of its elastic instability during uniaxial tension, which lies at approximately ε_m = 15% with c/a ≈ 1.16 and Ω/Ω_{exp} ≥ 0.95 (Ω_{exp} denotes the experimental atomic volume of bcc Fe). Further evidence is given by Tsetseris\textsuperscript{56} and Friák et al.\textsuperscript{57} which published minimum energy contour plots with respect to various magnetic orders (FM, AFM, and DAFM order by Friák et al. and non-collinear magnetism via a spin spiral formalism by Tsetseris) as a function of the bct geometry thereby defining magnetic phase boundaries between different magnetic states. According to both references, FM order is the predominant magnetic order in the configuration space for c/a ≤ 1.25 and Ω/Ω_{exp} ≥ 0.95. Both references hence indicate that the point of elastic instability for Fe reported by Clatterbuck et al. is indeed located far from the borderline of FM order towards any other investigated magnetic ground state order. Hence, here we assume that Fe and also the present Fe-rich binary alloys stay FM during the deformation process.

The ideal tensile strength σ_m corresponding to the strain ε_m from our and other calculations in [001] direction for iron are listed in Table I. It can be seen that the three projector-augmented wave (PAW) works\textsuperscript{1,18,19} show similar stress values, however scatter somewhat in ε_m. Namely, Clatter et al.\textsuperscript{1} reported a value of σ_m = 12.6 GPa at ε_m = 15% and Liu et al.\textsuperscript{19} gave a value of σ_m = 12.4 GPa at ε_m = 14%. Furthermore, the two σ_m values obtained by the all-electron full-potential linear augmented plane wave (FP-LAPW) method differ by 1.5 GPa (~ 11%). Compared to these theoretical full-potential data, the EMTO result for the stress of Fe is slightly smaller but still in reasonably good agreement. We obtained c/a ≈ 1.18 and Ω/Ω_{exp} ≈ 1.04 for the point of instability of Fe in agreement with Clatterbuck et al.\textsuperscript{20} Finally, we computed that the bct to orth branching occurs at ε = 19% well above ε_m in accordance with Ref. 1.

On the experimental side, the only attempt to measure the ideal tensile strength of Fe was by Brenner\textsuperscript{3} who tested Fe whiskers for tension was measured to be the [001] direction. The ITS of these Fe whiskers at room temperature was measured to be approximately 5 GPa. Compared to the theoretical data, the experimental value seems to be considerably lower. However, the observed failure initiated at the surface and, therefore, the measured value cannot be considered to represent bulk strength.

Based on the above results, we concluded that our theoretical tool is able to describe the ITS of bcc Fe with sufficiently high accuracy.

### Table I. The ideal tensile strength σ_m and the corresponding strain ε_m from our and published computations in [001] direction for a pure iron crystal. FP-LAPW stands for full-potential linearized augmented plane wave.

| element | method            | direction/[001] | σ_m (GPa) | ε_m (%) |
|---------|-------------------|----------------|-----------|---------|
| Fe      | EMTO              |                | 11.0      | 14      |
| Fe      | PAW Ref. 1        |                | 12.6      | 15      |
| Fe      | PAW Ref. 18       |                | 12.4      | 16      |
| Fe      | PAW Ref. 19       |                | 12.4      | 14      |
| Fe      | FP-LAPW Ref. 20   |                | 14.2      | 15      |
| Fe      | FP-LAPW Ref. 21   |                | 12.7      | 15      |

B. Ideal strength of Fe-based alloys

In the following we turn to bcc Fe-based alloys and investigate the effect of alloying elements M=Cr, Ni, Al, Co, Mn, and V on the ITS of Fe_{1-x}M_x random solid solutions. The selected solute atoms are common in commercial Fe-based steel alloys and they represent simple metal (Al), nonmagnetic (V) and magnetic (Cr, Co, Ni, and Mn) transition metals. The total concentration of these solutes was varied in the range from 0 to 10% except for Mn which the maximum concentration was 5%. The theoretical equilibrium lattice parameters of Fe_{1-x}M_x (M=Cr, Ni, Al, Co, Mn and V) random alloys are displayed in Table II. We can see that compared to pure Fe, all alloying elements increase the lattice constant. Our computed lattice constants practically reproduce the earlier results from Ref. 28.
Figure 1 shows the composition dependence of the ITS of binary bcc Fe-based random alloys along the [001] direction and the corresponding numerical data for selected compositions are listed in Table II. The calculated ideal strength is found to increase with Cr, Co and V and decrease with Ni and Al addition to Fe. For instance, when 10% Ni or Al are added to the Fe matrix, the ITS reduces by 10% Cr, Co, or V is added to bcc Fe, the ITS of Fe increases by 1.4, 0.8 and 2.4 GPa, respectively. If however 10% Ni or Al are added to the Fe matrix, the ITS reduces by 1.5 GPa. For Mn, first the ITS increases weakly with increasing Mn amount below 2.5%, i.e., from 11.0 GPa to 11.3 GPa, then reduces by 0.3 GPa when up to 5% Mn is added to Fe compared to pure Fe. According to Fig. 1, it is clear that Al, Ni, and V show the strongest average alloying effect (∆σ_m/∆x) on the ITS of bcc Fe, whereas Mn, Ni and Cr produce intermediate alloying effect.

### TABLE II. Theoretical (EMTO) lattice parameters a(x) (in Å) calculated for the ferromagnetic bcc Fe_{1−x}M_x alloys as a function of composition. For pure Fe, the value is a(0) = 2.829 Å.

| x    | Fe-Cr | Fe-Co | Fe-V | Fe-Ni | Fe-Al | Fe-Mn |
|------|-------|-------|------|-------|-------|-------|
| 2.5  | 2.843 | 2.837 | 2.842| 2.843 | 2.844 | 2.839 |
| 5    | 2.849 | 2.842 | 2.849| 2.852 | 2.853 | 2.843 |
| 7.5  | 2.850 | 2.845 | 2.850| 2.858 | 2.860 |       |
| 10   | 2.849 | 2.848 | 2.858| 2.861 | 2.866 |       |

We also considered the possibility of a branching from the primary bct deformation path to the secondary orthorhombic deformation path for the present Fe-based alloys. Based on these additional calculations, we can exclude a bifurcation from the primary bct deformation before the ideal strength is reached, i.e., for all alloys considered here the branching occurs at strains larger than ε_m.

### IV. DISCUSSIONS

#### A. Failure of the structural energy difference model for ITS

Understanding the alloying effects on the ITS of Fe-based alloys is highly desirable. To this end, we start from a previously established simple model based in structural energy differences. For binary and ternary vanadium based V_{1−y−z}Cr_yTi_z random solid solutions, 0 ≤ y + z ≤ 0.1, we established a qualitative correlation between the change of the ITS due to alloying and the change of the fcc-bcc structural energy difference (SED) of the alloy.22 Accordingly, the maximum stress (σ_m) was approximated by σ_m^{SED} along the [001] direction defined as

\[
\sigma_m \approx \sigma_m^{SED} = \frac{1}{\Omega_{bcc}} \frac{\Delta E_{SED}}{\Delta \epsilon}, \tag{3}
\]

where ΔE^{SED} denotes the SED at fixed volume (here of the bcc ground state, Ω_{bcc}) and Δε is the strain at constant volume necessary to transform the bcc lattice into the fcc lattice along the Bain transformation (Δε ≈ 0.260).

Equation. (3) is based on the fact that the fcc structure corresponds to the nearest maximum to the bcc phase of the uniaxial strain energy curve.1,19–21 Thus, the uniaxial strain energy must level off to the fcc-bcc energy difference, which implies a limitation on the maximum stress since it restricts ΔE(c; [001]) to the SED within the strain interval to accomplish the transformation from bcc to fcc, i.e., the ratio ΔE^{SED}/Δε is bounded.

The alloying trend is captured by Eq. (3) if there is a correlation between the change of the ITS as a function of concentration, ∆σ_m(x), and the change of the fcc-bcc SED, Δ(ΔE^{SED})(x). The prefactor 1/Ω_{bcc} is weakly concentration dependent and does not change the conclusions drawn here. We show in the following that the correlation suggested by Eq. (3) fails for the bcc FM Fe-based alloys as opposed to the nonmagnetic V_{1−y−z}Cr_yTi_z alloys.22

First, we assumed a FM state for both fcc Fe and the Fe-based alloys, since the FM fcc state of Fe was shown to be the nearest maximum of the uniaxial strain energy curve.1,19–21

![FIG. 1. (Color online) The ideal strength of Fe-based alloys as a function of composition.](image-url)
TABLE III. The ideal tensile strength $\sigma_m$, corresponding strain $\epsilon_m$ from our calculations in [001] direction for iron-based alloys.

| composition | $\sigma_m$ (GPa) | $\epsilon_m$ (%) | $\sigma_m$ (GPa) | $\epsilon_m$ (%) | $\sigma_m$ (GPa) | $\epsilon_m$ (%) |
|-------------|------------------|------------------|------------------|------------------|------------------|------------------|
| Fe-Cr       | 12.1             | 14.0             | 11.1             | 14.2             | 11.9             | 14.8             |
| Fe-Co       | 12.4             | 14.7             | 11.5             | 15.2             | 12.6             | 15.3             |
| Fe-V        | 12.4             | 14.5             | 11.7             | 14.9             | 13.2             | 15.3             |
| Fe-Ni       | 10.9             | 14.3             | 10.5             | 14.7             | 11.3             | 14.6             |
| Fe-Al       | 10.6             | 14.3             | 10.2             | 14.6             | 10.7             | 14.4             |
| Fe-Mn       | 10.1             | 13.6             | 9.7              | 14.4             |                 |                  |

Figure 2 displays $\Delta \sigma_m(x)$, obtained from the values in Table III, as a function of $\Delta (\Delta E_{\text{SED}})(x)$ calculated with EMTO-CPA. In figure, the alloying effect was obtained by increasing the concentration of the solute from 0 % to 5 %. We can see that Ni, Mn, and Al decrease the ITS and also decrease the SED, however, Co, Cr, and V increase the ITS but decrease the SED. We also investigated the correlation between $\sigma_m$ and $\Delta E_{\text{SED}}$ increasing the concentration of the solute from 5 % to 10 %, however the result is qualitatively identical to the one depicted in Fig. 2. From these results, we infer that the anticipated correlation between the ITS and the FM SEDs following Eq. (3) can not capture the observed alloying trend of $\sigma_m$.

Next we tried to establish a correlation between the PM SEDs obtained from paramagnetic (PM) fcc Fe$_{1-x}$M$_x$ alloys and their FM bcc phases. Using the above described procedure and a concentration increase of the solute from 0 % to 5 %, we plotted the stress change versus the PM SED change in Fig. 3. From that figure, it can be clearly seen that Ni and Mn decrease the ITS and likewise decrease the SED, while Cr, Co, and V increase the ITS as well as they increase the PM SED. However, FeAl is outlying as the ITS decreases with Al, but the PM SED increases with Al. Assuming a paramagnetic fcc state thus captures somewhat better the observed alloying trends than a FM fcc but the correlation dictated by Eq. (3) is still not perfect.

One possible reason why Eq. (3) is not a good estimate for the alloying trend of $\sigma_m$ for Fe alloys may be related to the different employed deformations paths. Along the unconstrained primary deformation path of tensile stress, the volume of the unit cell can change and $a$ is determined from Eq. (2). Fcc-bcc SEDs on the other hand
we expect that the correlation between
Since both values were obtained for the same strain path, that the above failure can
magnetism and the structure in Fe along the deforma-
constant volume for each Fe-alloy is the one of its theo-
as a function of strain for fixed unit cell volume. The
volume deformation, i.e., the maximum stress according
computed an auxiliary ideal stress assuming a constant
is comparable for both strain paths. That was indeed the
case for nonmagnetic V-based random alloys.

B. Magnetic effects on the ITS

To achieve a better understanding of the matter, we
computed an auxiliary ideal stress assuming a constant
volume deformation, i.e., the maximum stress according
to Eq. (1) was deduced from the total energy computed
as a function of strain for fixed unit cell volume. The
constant volume for each Fe-alloy is the one of its theo-
rical equilibrium volume (Table II). The so-calculated
maximum stress at constant volume, \( \sigma^\Omega_m \), with maximum
strain, \( \epsilon^\Omega_m \), is then correlated to FM \( \Delta E^{\text{SED}} \) from Eq. (3).
Since both values were obtained for the same strain path, we expect that the correlation between \( \sigma^\Omega_m \) and \( \Delta E^{\text{SED}} \) significantly improves for all alloys, despite possible in-
terference from magnetism.

First, \( \sigma^\Omega_m \) as an approximate to the ideal strength of
Fe-based alloys as a function of the alloying elements is
presented in the following section, that the above failure can
indeed be originated in the effect of magnetism.

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By comparing Fig. 4 with Fig. 1, it is immediately ev-
ident that the ideal strength of Fe is most significantly
affected by the fixed volume constraint, i.e., it increases
from 11.0 GPa to 16.0 GPa. This is unlike the Fe-alloys
with moderate solute concentrations, where the ideal
strength increases are considerably smaller the higher the
solute concentration are, e.g., we obtained an increase
from 13.4 GPa to 15.1 GPa for Fe-10V.

An answer to the observed correlation may be given
by considering magnetism in Fe and its alloys. In the
following we chose Fe-10V as a representative of all in-
vestigated binary alloys. The total energy and the spin
magnetic moment of Fe are opposed to those of Fe-10V in
Fig. 6, where we plotted both quantities as a function of the
tetragonal axial ratio \((c/a)\) and the Wigner-Seitz radius, \(\omega\). We also displayed the corresponding uniaxial
deformation path in the range from \(\epsilon = 0 \ldots \epsilon_m\).

As visible from the contour plots, the magnetic mo-
ment increase of Fe along the deformation allowing for a volume change from \( \epsilon = 0 \ldots \epsilon_m \) is much stronger than the one of Fe-10V; the numbers read 0.27 \( \mu_B \) and 0.09 \( \mu_B \) for Fe and the Fe-10V alloy, respectively. These numbers are in contrast to the deformation at constant volume (in the range \( \epsilon = 0 \ldots \epsilon_m^{(2)} \)), where the changes are 0.09 \( \mu_B \) for Fe and 0.03 \( \mu_B \) for Fe-10V. That indicates that the increase of the atomic volume has a more pronounced influence on the relaxation of the magnetic moment than the structural change \((c/a)\), a result which can be clearly associated with the contour lines in Fig. 6. It should be noted that \(|\epsilon_m^{(1)} - \epsilon_m^{(2)}|\) is at most 1.5% (for one and the same material), i.e., \( \epsilon_m^{(1)} \) is quite similar to \( \epsilon_m^{(2)} \) for Fe and the present Fe-alloys.

Now, alloying Fe with any of the solutes under investigation in this work increases the equilibrium volume (Table II). Unconstrained uniaxial tensile loading is also accompanied by an increase of the volume per atom, as depicted in Fig. 7 for Fe and for the Fe-based alloys with the highest considered solute concentrations. In the region of the maximum strains, both Fe and the Fe alloys have rather similar volumes as opposed to the situation at equilibrium. The volume change of Fe due to the deformation is thus distinctly larger than those of the Fe-based alloys. According to our numerical data (also Fig. 6), the larger volume increase of Fe is paralleled by a larger magnetic moment increase along the uniaxial deformation from equilibrium to \( \epsilon_m \), despite the fact that Fe contributes only by a factor of \( 1-x \) to the magnetic moment of the alloys.

The comparatively large increase of the magnetic moment in Fe along the uniaxial deformation path with unconstrained volume and the pronounced difference between \( \sigma_m^{(1)} \) and \( \sigma_m \) (5 GPa) may, at least in parts, be related. We recall, that both the increase of the magnetic moment and the difference \( \sigma_m^{(1)} - \sigma_m \) of all Fe-alloys are smaller than the values of Fe. To substantiate this correlation, we recalculated the ITs for the previously determined unconstrained strain paths but with fixed magnetic moments, i.e., the magnetic moments were not allowed to relax to self-consistency. We employed the respective ground state magnetic moments of Fe and the Fe-V alloys.

Fixing the magnetic moment increases the resulting computed strengths, but the increase is strongly diminished with higher solute concentration, e.g., approxi-
V. CONCLUSIONS

The ideal tensile strengths of bcc ferromagnetic Fe and Fe$_{1-x}$M$_x$ (M=Cr, Ni, Al, Co, Mn, and V) random alloys in the [001] direction have been investigated using the all-electron exact muffin-tin orbitals method in combination with the coherent-potential approximation. The present calculated ideal strength value of Fe and the branching point from the primary bct deformation path to the secondary orthorhombic deformation path of Fe agree well with previously published results, which thus confirms that our methodology has the accuracy needed for such kind of calculations. For the Fe-based alloys, we found that the ideal strength increases with increasing concentration of Cr, Co, and V and decreases with Ni and Al addition into pure Fe. Mn shows a non-monotonous alloying behavior. Unlike the nonmagnetic bcc V-based alloys investigated in our previous paper, constant volume fcc-bcc structural energy differences can not entirely capture the alloying effect on the ideal tensile strength for the FM bcc Fe-based alloys. By calculating auxiliary ideal strengths assuming a constant volume deformation ($\sigma_{m}^{\Omega}$) and fixed-spin moment calculations along the (kept unaltered) tetragonal deformation paths, we showed that mainly the interplay between the volume increase and magnetic moment increase along the tetragonal deformation paths lead to a failure of the correlation between $\sigma_{m}$ and $\sigma_{m}^{\text{SED}}$.

The present results offer a consistent starting point for further theoretical modeling of the micro-mechanical properties of Fe-based alloys. Based on these achievements, we conclude that the EMTO-CPA approach provides an efficient and accurate theoretical tool to design the mechanical strength of ferromagnetic bcc random solid solutions. Nevertheless, in such applications one should always monitor the basic muffin-tin and single-site CPA errors and make sure that they remain at acceptable level as a function of the lattice distortion and chemical composition.

VI. ACKNOWLEDGEMENTS

The Swedish Research Council, the Swedish Steel Producers’ Association, the European Research Council, the China Scholarship Council and the Hungarian Scientific Research Fund (research project OTKA 84078), and the National Magnetic Confinement Fusion Program of China (2011GB108007) are acknowledged for financial support. S.S. gratefully acknowledges the Carl Tryggers Stiftelse for Vetenskaplig Forskning and Olle Erikssons stiftelse for materialteknik.
