Decisive role of magnetism in the interaction of Chromium and Nickel solute atoms with $1/2\langle 111 \rangle$ -screw dislocation core in body-centered cubic Iron.

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Abstract

Resistance to swelling under irradiation and a low rate of corrosion in high temperature environments make Fe-Cr and Fe-Cr-Ni alloys promising structural materials for energy technologies. In this paper we report the results obtained using a combination of density functional theory (DFT) techniques: plane wave basis set solutions for pseudo-potentials and multiple scattering solutions for all electron potentials. We have found a very strong role of magnetism in the stability of screw dislocation cores in pure Fe and their interaction with Cr and Ni magnetic impurities. In particular, the screw dislocation quadrupole in Fe is stabilized only in the presence of ferromagnetism. In addition, Ni atoms, whose magnetic moment is oriented along the magnetization direction of the Fe matrix, prefer to occupy in core positions whereas Cr atoms, which couple anti-ferromagnetically with the Fe matrix, prefer out of the dislocation core positions. In effect, Ni impurities are attracted to, while Cr impurities are repelled by the dislocation core. Moreover, we demonstrate that this contrasting behavior can be explained only by the nature of magnetic coupling of the impurities to the Fe matrix. Specifically, Cr interaction with the dislocation core mirrors that of Ni if the Cr magnetic moment is constrained to be along the direction of Fe matrix magnetization. In addition, we have shown that the magnetic contribution can affect the impurity-impurity interaction at distances up to a few Burgers vectors. In particular, the distance between Cr atoms in Fe matrix should be at least 3-4 lattice parameters in order to eliminate finite size effects.

Keywords: Screw Dislocation, Magnetic Moment, Ferromagnetism

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1. Introduction

Resistance to radiation-induced swelling and a low corrosion rate in high temperature environments **make** Fe-Cr and Fe-Cr-Ni alloys promising structural materials for energy technologies. High mechanical stability under deformation conditions is the main demand on structural materials. Deformation properties of bcc metals/alloys, especially at a low temperature, are known to be controlled by the intrinsic core properties of their $\frac{1}{2}\langle 111 \rangle$ -screw dislocations. The origin of the specific plastic behavior of bcc metals is related to the non-planar extended core configuration of screw dislocations [1-3]. In any given material, the structure and properties of the screw dislocation core result from an interplay between crystallographic and bonding properties. **The distinction** between these two aspects and recognition of their relative significance are important **to a** fundamental understanding of plasticity in different bcc metals [4]. While crystallographic aspects can be studied by other atomic scale techniques, the bonding effects, especially in complicated cases where strong magnetism is involved, requires a proper way of accounting for the electronic bonding – such as in density functional theory (DFT) based methods.

Ferritic alloys, i.e. Fe-based alloys with a bcc structure, are well known to be highly resistant to radiation effects, such as swelling and damage accumulation, particularly compared to austenitic alloys (Fe-based alloys with fcc structure) [4-10]. In addition, high chromium contents (9–12 wt.%) are known to provide good corrosion resistance [11]. For these reasons, high Cr ferritic/martensitic steels are promising structural materials for key components in future nuclear energy options [12,13]. Nickel is used in low-alloy steels to improve strength and toughness. Although, the knowledge of its effect on radiation resistance in ferritic steels is rather limited, there is clear evidence that Ni affects Cu-precipitate evolution in bcc pressure vessel steels [14,15], dislocation loop populations [16], and mechanical properties [17]. In some irradiation environments, Ni may promote swelling due to helium production by nuclear transmutation reactions [12].

Pure Fe and Fe-Cr and Fe-Ni materials represent a great challenge for computational materials science because the magnetism of constituent elements affects the properties of

the alloys in a complex way [18]. As a result, only a few of the current DFT-based methods can robustly treat these materials with predictive accuracy.

The $1/2 \langle 111 \rangle$ -screw dislocation in a bcc lattice has been extensively investigated before using DFT methods [19-30]. Three types of the dislocation cores were reported: the so-called easy, hard and split cores [31-33]. The ground state of the $1/2 \langle 111 \rangle$ -screw dislocation in pure bcc metals corresponds to the symmetric, non-degenerate easy core structure. However, it can be affected locally by bond changes due to impurities. As was demonstrated recently, alloying of W with Re [27] or any transition metal from the VIIIA group of the periodic table [23] breaks the symmetry of the easy core configuration. A similar modification was obtained in alloying bcc Fe with significant amounts of Co [28]. So far, the effects of substitutional atoms on dislocation core structure were primarily investigated using the virtual crystal approximation (VCA) [34]. Unfortunately, the VCA only provides a gross estimate of the average modification of electronic structure due to alloying [23, 27, 28], in particular, the filling of the d -states [23]. An alternate approach is the construction of supercell models containing screw dislocations in which solute atoms are substituted for host atoms, either in the dislocation core or at some appropriate distance from it (see for example publications [24, 29]). Unfortunately, supercell models suffer from restrictions imposed by the limits on the maximum number of atoms realistically accessible to conventional DFT codes that limit the thickness of the modeling cell along the dislocation line to a single Burgers vector. One Burgers vector thickness of a sample consists of three atomic planes in $[111]$ direction. For impurity studies, the size limitation then implies that the dislocation core interacts not with an isolated impurity atom but with a chain of atoms along the dislocation line that are only separated by one Burgers vector.

An alternative approach to direct supercell based DFT modeling is to first map results of DFT calculations on to a tight binding model Hamiltonian, which then allows simulations of much larger supercells. Recently, this kind of method has been used to model dislocation core structure and migration barriers in bcc iron within the framework of Bond Order Potential (BOP) techniques [35]. While this method is successful, the results of such

simulations are in overall agreement with direct DFT calculations themselves. Given that the BOP approach requires a series of fitting parameters, the extension of this method to more complex multicomponent systems such as studied here requires verification. As a result, in this work, we take the view that direct DFT approach is a good starting point for the investigation of the interaction of magnetic impurities with a dislocation core, provided that attention is paid to consequences of the effects of using smaller supercells than those accessible using the BOP approach. In reverse, they also provide insights into the underlying physics (bonding, magnetism etc.) that such model approaches must be of sufficient fidelity to capture.

In this paper we present the results of atomistic studies of screw dislocation properties using a combination of DFT techniques that allow us to model the interaction between a dislocation core in bcc iron and “individual” Cr and Ni impurity atoms in a realistic way. The set of properties considered includes the $1/2\langle 111 \rangle$ -screw dislocation core structure, its interaction with impurity atoms and an investigation of the decisive role of magnetism in determining whether or not the impurity interaction is attractive or repulsive.

The remainder of the paper is organized as follows. In section 2 we briefly review the computational approach. In Section 3.1 we discuss magnetic ordering effects on the stability of core structure of a screw dislocation in pure Fe. The interaction of a Ni or Cr solute atom in Fe with the dislocation core and the role of magnetism are described in Section 3.2. Section 3.3 presents results of studies of the effect of increasing the impurity separation along the dislocation core direction on the strength of the impurity-dislocation interaction and the minimal periodicity required to obtain the isolated impurity limit. Finally, the conclusions are given in section 4.

2. Computational approach

The electronic structure and structural relaxations have been calculated using the plane wave based DFT method as implemented in the Quantum ESPRESSO (QE) package [36]. We employed an ultrasoft pseudo-potential [37] optimized in the RRKJ scheme [38]. The

generalized gradient approximation (GGA) exchange-correlation functional with the Perdew, Burke, and Ernzerhof [39] parameterization was used. The Brillouin zone (BZ) summation was carried out over a $1 \times 2 \times 8$ BZ grid. Electronic smearing with a width of 0.02 Ry was applied according to the Methfessel-Paxton method. The plane wave and the charge density energy cutoffs were chosen at 43 and 334 Ry, respectively, which provides an accuracy of 0.2 mRy/atom. The atomic structure was optimized until the forces on all atoms dropped below 0.001 Ry/A. The lattice constant used in this investigation is determined from the equilibrium volume for pure bcc Fe, 2.89 Å.

We used a periodic quadrupolar arrangement for a $1/2\langle 111 \rangle$ screw dislocation [40] in a cell with basis vectors $\vec{b}$, and , where], and]. An appropriate choice of lattice vectors [41] reduces this quadrupole cell to half the size, having basis vectors of 2, and and 135 atoms. This unit cell contains only two dislocations with opposite Burgers vectors and a thickness of one Burgers vector as shown in **Fig. 1**. It was demonstrated earlier that this cell size is large enough to adequately reproduce the energetics of screw dislocations [19–23, 41].

Atomic scale magnetic properties of the optimized structures were further investigated using the Locally Self-consistent Multiple Scattering method (LSMS) [42], an all-electron, real space approach, based on multiple scattering theory within the framework of density functional theory (DFT) and local spin density approximation (LSDA)[43]. The method permits the calculation of electronic structures for systems comprising 10^3 - 10^5 atoms thanks to its built-in scalable parallelism [22,44]. Use of the LSMS allowed us to extend the size of the dislocation structures beyond what plane wave based codes routinely permit, therefore allowing us to model interactions between the dislocation core and individual solute atoms that are separated by $(n = 1,2,3,4)$ periodic repeats along the dislocation core direction. In previous DFT attempts it was possible only to model interactions with a single repeat, which essentially represents a row of solute atoms parallel to the dislocation core direction. This is especially important for considering magnetic effects on defect-defect interactions on be long ranged thereby extending beyond several Burgers

vectors and many lattice parameters.

3. Results

3.1. Magnetic state effects on the screw dislocation core structure in bcc Fe

The experimentally observed ground state of Fe is bcc ferromagnetic (FM). Fe in the fcc structure is paramagnetic within the temperature range of thermodynamic stability (1184–1665 K). It was clearly demonstrated that ordering of Fe in a bcc structure at low temperature is caused by magnetism [45, 46]. According to its position in the row of transition metals, Fe with six *d*-electron states occupied, should crystallize in an hcp structure, as do *4d* Ru and *5d* Os that are in the same column of the periodic table [47-49]. The magnetism and energetics of bcc Fe have been widely investigated using *ab initio* electronic structure methods [50-53]. Thermodynamic arguments based on measured heats of formation and FeX binary phase diagrams also support the role of magnetism in stabilizing the bcc phase [54]. *Ab initio* results show that non-magnetic (NM) bcc Fe is unstable to transformation to fcc. Thus, it is clear that the stability of bcc Fe depends critically on the magnetic state. Here, we address the role of magnetism in the stability of $1/2\langle 111 \rangle$ screw dislocations by first constructing a relaxed dislocation quadrupole using *ab initio* methods (QE) based on three very different treatments of the magnetic state within DFT, namely FM, NM, and antiferromagnetic (AFM).

The results for the structure of the $1/2\langle 111 \rangle$ -dislocation quadrupole in FM, NM and AFM magnetic states are presented in **Fig. 1** (left to right accordingly). It should be mentioned that the full quadrupole of a screw dislocation with total Burgers vector equal to zero is a metastable configuration and is separate from the ground state, which is the perfect bcc lattice, by the barrier of ~ 40 meV per Burgers vector [25, 30].

The circles in **Fig. 1** represent Fe atoms looked at from the $\langle 111 \rangle$ direction and the dislocation structure is illustrated by differential displacement (DD) maps [55]. On a DD map the displacement of an atom in the $[111]$ direction relative to a neighbor is plotted as an arrow connecting the atom with its neighbors. The length of an arrow is normalized so

that arrows connecting two atoms correspond to displacement by $b/3$, where b corresponds to length of a Burgers vector thus indicating the dislocation core. The sum of the all arrows in the circuit around a dislocation gives the Burgers vector. In agreement with previous results for bcc metals [19, 21, 23-27, 30], we obtained the symmetric non-degenerate configuration for a screw dislocation core in Fe FM state (**Fig. 1a**). The suppression of magnetism in the NM state leads to recombination of dislocation cores with opposite Burgers vectors (**Fig. 1b**). Because of the finite size supercell, the reduced dipole configuration described above cannot recover the perfect bcc structure after the recombination of dislocation cores and a small remaining misfit can be seen in **Fig. 1b**. This recombination is the result of a general loss of stability of the Fe bcc lattice in the NM state when using the GGA exchange correlation functional. It was demonstrated earlier [56-58] that conventional methods find the NM state of bcc iron to be mechanically unstable, e.g. the elastic constant c' is negative and there are imaginary phonon dispersion braches. We also obtained a very similar core recombination for AFM magnetic ordering (**Fig. 1c**), which is again due to the negative c' value. This sensitivity of dislocation structure demonstrates the extreme importance of the correct description of magnetism in pure iron and iron-based magnetic alloys. Moreover, the magnetic state change can lead to modification of dislocation structure and mobility. The instability of NM and AFM bcc iron lattice can be overcome by either application of model methods which include spin fluctuations [57], disordered local magnetic moments (DLM) [58-59] or modern dynamical mean field theory approaches [60-62]. These approaches preserve the positive value of c' and reproduce the experimentally observed significant reduction of c' at T_c (the experimental reduction of c' at T_c is close to 60 % [63]). It looks very likely that such a significant reduction of c' at temperatures close to T_c will also lead to modification of the screw dislocation core; however, these types of calculation are currently too time-consuming to be applied to systems containing 100's of atoms.

3.2. Interaction of Ni and Cr solute atoms with $\frac{1}{2}\langle 111 \rangle$ -screw dislocation in bcc Fe

In order to model interactions between the screw dislocation core and solute atoms, we substituted Fe atoms by either Ni or Cr atoms at various sites. The DD map of the

dislocation presented in Fig. 2 shows four impurity positions that were investigated by a blue solid circles: Fig. 2a in the full modeling cell; Fig. 2b in an enlarged area around the dislocation core. The impurity positions are enumerated from 1 (in core) to 4 (off core); the latter being as far away from the core as possible within the current simulation cell. We observed that the substitution of a Fe atom by either a Ni or Cr atom does not produce any significant modification of the core structure within the accuracy of the DD map plot. This is because the low concentration of Ni (Cr) impurities in Fe does not lead to substantial changes of associated with *d*-electron bonding, which is in contrast to tungsten based alloys [23] where alloying with VIIIA elements results in more directional bonding and changes symmetry of the dislocation core [23,27]. The change in total energy for the core and off-core positions of the impurity atoms is shown in Fig 3. Here, the energy of systems in the furthest (4-th) off-core position is chosen as the zero of energy. At this distance the impurity atom is no longer influenced significantly by the dislocation core and the formation energy of the impurity atom is closest to its value in bulk.

To obtain accurate energetics, we first relax the dislocation quadrupole in pure Fe, then substituted a Fe atom at some site specified by an impurity and relax the system again. As can be seen from the figure, the interaction of Ni atoms with the dislocation core is attractive and equal to -17 meV. Interestingly, the interaction of Ni atoms in positions 2 and 3 with core is positive. In contrast, the Cr impurity at the core has energy of 78 meV and decays with distance (positions 2 and 3), thus is repelled by the dislocation core. Such a large difference between the behavior of Ni and Cr impurities cannot be described by simple elastic interactions because a screw dislocation core does not produce a hydrostatic pressure component and therefore does not interact with any dilation center, at least within linear elasticity. Moreover, the values of the dilatation volume for Cr and Ni substitutes estimated in the 2x2x2 supercell are quite small, 0.4 and 0.3 % of the Fe equilibrium atomic volume respectively; as a result this contribution can be neglected. On the other hand, analysis of magnetic structure shows that the magnetic moment of the Ni substitution is ordered in the same direction as the moments of host Fe atoms (i.e. ferromagnetically), whereas that of Cr atom is ordered in the opposite direction (i.e. antiferromagnetically).

To demonstrate that magnetism and magnetic ordering are the cause of this contrasting energetics, we used the LSMS code to create an artificial Cr atom that has ferromagnetic coupling with the Fe matrix. Because the current LSMS implementation does not return forces we cannot perform ionic relaxation. Therefore, we first investigated the substitution atom's relaxation energy and its contribution to the binding energy with the dislocation quadrupole. Using QE, we ran the same systems with Ni (Cr) impurity with and without ionic relaxation. We found that the contribution of relaxation to the binding energy is less than 0.2 % (-0.03 eV) for Ni and ~10 % (-9 meV) for Cr atoms. We therefore believe that the ionic relaxation around Ni and Cr substitutions can be safely neglected in LSMS calculations. Our result for the binding energy obtained with the LSMS approach is -12 meV for the Ni impurity and 60 meV for Cr. We attribute the majority of 15% difference to the different exchange-correlation functionals used in the LSMS and QE calculations; namely LDA versus GGA.

To investigate the importance of the different magnetic states of Ni and Cr impurities we use the LSMS method to manipulate the local magnetic moment by applying an additional constraining potential on the Cr atom to change the exchange splitting between the majority and minority spin states. In this way it is possible to tune the Cr moment to some prescribed value. In other words, the magnetic state of the Cr atom can be altered so that it eventually achieves ferromagnetic rather than anti-ferromagnetic coupling with Fe. At each value of exchange splitting the Fermi energy is recalculated in order to preserve total number of valence electrons and ensure overall charge neutrality. The result is shown in **Fig. 4** where the difference between binding energies of two systems, one containing Cr impurity at the core site and the other at the off-core (bulk) site, is shown as a function of constrained magnetic moment of Cr impurity. At the Cr ground state moment of $-1.5 \mu_B$, the off core is preferred. As the constraining field is increased, the magnetic moments at the core site eventually becomes positive, implying that the magnetic coupling of Cr with the host matrix is now ferromagnetic. When the core-site Cr moment reaches $+0.75 \mu_B$, which is the value of magnetic moment of a substitutional Ni atom, the in core position is clearly favored, reversing the interaction picture observed for the ground state where the moment is $-1.5 \mu_B$. The total energies of a Cr impurity at the sites 1,2,3,and 4 (red line) relative to

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4 impurity in bulk (taken as site 4) are shown in **Fig. 5** when the constrained magnetic
5 moment is equal to $+0.75 \mu_B$ at each site. As can be seen, the ferromagnetically coupled Cr
6 at the dislocation core is even more stable than the Ni impurity, clearly demonstrating that
7 the difference in interaction behavior of Ni and Cr solute atoms with the dislocation core is
8 driven by magnetism.
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14 3.3. Ni/Cr: isolated impurity vs. impurity row

15 Due to the simulation supercell size limitations, *ab initio* models of dislocations usually
16 consider a periodic repeat along the dislocation line of only a single Burgers vector
17 (namely, three (111)-atomic planes). This significantly reduces the size of the modeling
18 cell, e.g. to 135 atoms in the current case, and works reasonably well for modeling of pure
19 metals. In this setting however, placing even a single impurity atom in the cell in fact
20 introduces an infinite chain of impurity atoms along the dislocation line separated by one
21 Burgers vector. This is clearly very different from the dislocation core interacting with an
22 individual impurity atom. To address this finite size effect a combination of DFT techniques
23 was used. An extended supercell is prepared from the initial QE-optimized simulation cell
24 that contains the screw dislocation quadrupole in pure iron of the thickness of one Burgers
25 vector by replicating it along the Burgers vector direction. This relaxed configuration was
26 then used within the LSMS method to study the effects of increasing the periodicity along
27 the dislocation line. A single Ni (Cr) impurity was then created by substituting a Fe atom at
28 a specific site. Only the electron distribution, not the ionic structure was optimized due to
29 limitations in the current version of the LSMS. As demonstrated above, this introduces
30 about 0.2% and 10.0% uncertainty into the binding energy value for Ni and Cr impurities,
31 respectively. The result for the binding energy as a function of the dislocation line length,
32 which is the same as distance between impurities in the chain along the [111] direction, is
33 shown in **Fig. 6**. The binding energy of Ni at the core site depends weakly on the sample
34 thickness, whereas that for Cr interactions shows a threefold reduction resulting from the
35 thickness of the sample parallel to the dislocation line. The later saturates only at distances
36 above $\sim 25 \text{ \AA}$ (i.e. three Burgers vectors). The significant difference in the energy of Cr-Cr
37 interactions is attributed to their magnetic coupling with the rest of the Fe matrix due to
38 the anti-ferromagnetic coupling of Cr with both surrounding Fe atoms and its own periodic
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images, thereby perturbing a larger region. In contrast, the effect of introducing a Ni impurity into the Fe-matrix appears to be much more localized; presumably thanks to its ferromagnetic coupling with the surrounding Fe atoms and its own periodic image.

These results demonstrate that in modeling of impurities that are anti-ferromagnetically coupled with the host matrix, one should take into account how far its effects extend. In the particular case of Cr impurities in Fe, this requires a supercell size of more than three Burgers vectors along the [111] direction of the dislocation core.

4. Conclusions.

We used combination of two DFT based techniques to study the interaction of Ni (Cr) substitution impurity with $1/2\langle 111 \rangle$ -screw dislocation to determine the effects of magnetism on this interaction. The following effects have been observed:

- Suppression of magnetism in bcc Fe leads to recombination of $1/2\langle 111 \rangle$ -screw dislocation quadrupole indicating the importance of magnetism for the stability of the dislocation core structure in Fe.
- Substitution of Fe by Cr or Ni leads to small relaxation of initial atom positions, which can be neglected.
- Energetically, a Ni atom favors the site at dislocation core, suggesting that Ni solute impurities will segregate near the core. In contrast, Cr favors the site away from the core, suggesting that Cr solute impurities will be segregated in the regions away from dislocation cores.
- The difference in segregation behavior of Ni and Cr atoms is driven by magnetism; Ni is ferromagnetically coupled with host Fe matrix whereas Cr is anti-ferromagnetically coupled. Creation of a fictitious constrained ferromagnetically coupled Cr atom results in behavior that is similar to Ni.
- The Cr-Cr interaction extends at least up to three Burgers vectors along the dislocation line. In fact, the interaction energy between two Cr atoms increases by a factor of 3 when the two atoms are separated by one Burgers vector as opposed to 3 Burgers vector. The Ni-Ni interaction decays within one Burgers vector.

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Figure captions:

Fig. 1. The [111] projection of the dislocation dipole unit cell, where atoms are shown by circles and the arrows corresponds to differential displacement, in a) ferromagnetic, b) nonmagnetic and c) antiferromagnetic bcc iron.

Fig. 2. DD map of the dislocation dipole unit cell with Ni/Cr atom impurities: a) full modeling cell with Cr or Ni substitution atom position shown by filled (blue on in color figures) circles and b) the enlarged figure of the region around dislocation core with enumerated positions of substitution atom. The substitution atom position numeration corresponds to the numeration in **Fig. 3**. The open circles correspond to Fe atoms and different colors correspond to three different planes.

Fig. 3. Total energy as a function of distance from the dislocation core for Cr (red) and Ni (blue) atoms. The zero distance corresponds to the core position and the energy of farthest impurity is chosen as zero energy. Results obtained from LSMS (solid lines) closely match with results from QE (dashed lines). Cr impurity strongly favors the site far from core, while Ni impurity favors the site at the core. Fe substitution sites are labeled as 1,2,3 and 4.

Fig. 4. Difference between binding energies of two systems, one containing Cr impurity at the off-core site and the other at the core, shown as a function of constrained Cr impurity magnetic moment. At ground state moment of $-1.5 \mu_B$, off core site is preferred. At the constrained moment value of $+0.75 \mu_B$, that of Ni moment at ground state, the core site is energetically favorable.

Fig. 5. The total energy as a function of distance for Cr (red) and Ni (blue) impurity from the dislocation core at constrained momentum value of $+0.75 \mu_B$ on Cr atom (*). The zero distance corresponds to the core position and the energy of farthest impurity is chosen as zero energy. Cr impurity now strongly favors the core site.

Fig. 6. Binding energy as a function of the distance between impurities along line of dislocation (supercell thickness).

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Dipole of screw dislocaions in bcc Fe

FM

NM