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Quantification of ferrite-martensite interface in dual phase steels: A first-principles study

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ABSTRACT

The ferrite-martensite interfacial energy and equilibrium interfacial length as a function of martensite carbon content are assessed using first-principles atomistic simulations. The weight percent of carbon in the martensite phase was implicitly varied from 0.6 to 1.8 wt percent by modifying the lattice constant of body-centered tetragonal (BCT) martensite according to Kurdjumov and Kaminsky's empirical expressions. With increasing carbon content, a decrease is found in both the interfacial energy and in the equilibrium distance between ferrite and martensite interfaces. Moreover, the Morse interatomic potentials between the atoms in the ferrite-martensite interface for four different martensite carbon contents are calculated, and the parameters of the Morse potential are correlated linearly with the martensite carbon content. In addition, the dissociation local strains during uniaxial loading in a direction normal to the interfacial plane are calculated from the interatomic potentials. The local strain at the interface needed for ferrite-martensite interface separation increases with increase in martensite carbon content. The fitted expressions can be used to predict the ferrite-martensite interfacial energy, equilibrium interfacial distance, dissociation local strain at the interface, and the Morse parameters as functions of martensite carbon content within the range of 0.6–1.8 wt percent. Furthermore, the introduced implicit method can potentially be used to study the mechanical properties of other materials with dopant impurities such as n-type and p-type semiconductors.

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1. Introduction

Dual-phase (DP) steels are promising materials for a wide variety of automobile parts due to their remarkable mechanical properties such as combined high strength and good ductility [1,2]. These properties are attributed to the microstructure of DP steels, which consists of hard martensite particles dispersed in a soft and ductile ferrite matrix. However, the application of DP steels is currently restricted due to their complex failure behavior, arising from their microstructure. Therefore, the effect of microstructural characteristics on the failure initiation of DP steels is an important topic and has been the subject of extensive research [3–5].

Two competing failure mechanisms, namely martensite cracking and ferrite-martensite interface de-cohesion, dominate failure initiation in DP steels [6]. Previous studies showed that

martensite volume fraction, martensite morphology, and ferrite grain size control which of these two mechanisms dominate in these materials [7–14]. However, investigations by Tasan et al. [15] revealed that both mechanisms can occur in conventional and modern DP steels, for which the martensite volume fraction is less than 50% and the ferrite grain size is less than 20 μm . Therefore, another parameter besides ferrite grain size and martensite content should be introduced as a controlling parameter for failure initiation in these materials.

In this work, martensite carbon concentration is introduced as the crucial additional parameter controlling the mechanical properties and failure initiation of DP steels. Thus, both failure mechanisms (i.e., martensite cracking and interface debonding) should, we believe, be formulated as a function of martensite carbon content. The Extended Finite Element Method (XFEM) with traction-separation (cohesive law) and cohesive zone models are typically used to simulate martensite cracking and ferrite-martensite debonding, respectively. We have previously formulated XFEM parameters controlling martensite cracking as a function of martensite carbon content for DP600 steels in microscale and

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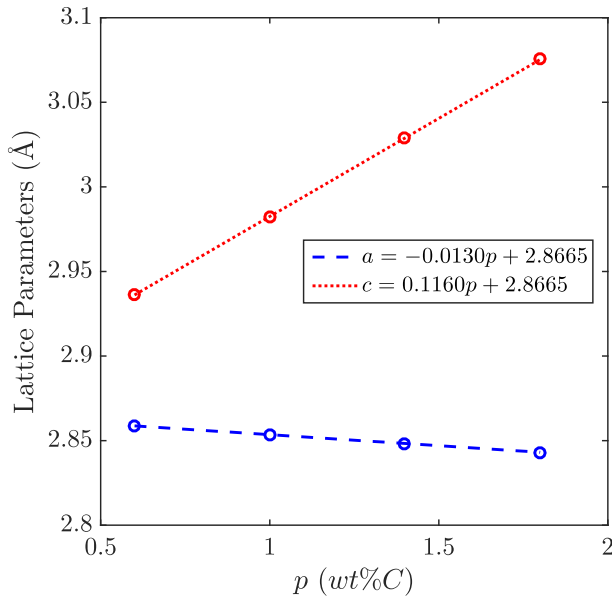


Fig. 1. The variation of the lattice parameters of high-carbon martensite ferrous with a body centered tetragonal (BCT) structure with respect to its carbon content. The linear regressions provided in Ref. [40] were used to obtain the lattice constants at the designated points [40].

provided simple equations for these parameters and validated them for various industrial DP steel grades with different chemistries, microstructures and mechanical properties [16]. Here, the cohesive zone model parameters are formulated as a function of martensite carbon content to simulate ferrite-martensite interface decohesion. It is expected that the results of this work will enable us to evaluate the dominant failure mechanisms for failure initiation in DP steels by calculating the critical energy for ferrite-martensite interface decohesion as well as martensite cracking.

Density functional theory (DFT) has been extensively used in studying metallic interfaces [17]. For example, Martin et al. used first-principles calculations of solid-solid interfaces to study conversion materials for lithium-ion batteries [18]. Moreover, Johnson et al. studied the structure, magnetism and adhesion at Cr-Fe interfaces using density functional theory [19]. Recently, Kazemiabnavi et al. utilized density functional theory to study the metallic electrode-liquid electrolyte interfaces in lithium-air batteries [20–25]. DFT methods have also been applied to study metallic iron surfaces such as surface relaxation [26] as well as surface magnetic moments [27] and have proven to be in good agreement with experiments. In a study by Hung et al. the adhesion between bulk-terminated BCC Fe (100) and Fe (110) interfaces was simulated in epitaxy and the maximum lattice mismatch possible for epitaxial growth was determined using DFT with the plane wave pseudopotential approximation [28].

The current work is a preliminary study to quantify ferrite-martensite interfacial parameters as a function of martensite carbon content in DP steels. We utilize density functional theory (DFT)

to calculate ferrite-martensite interfacial energy and equilibrium interfacial length as a function of martensite carbon content. Moreover, the interatomic potentials between the atoms in the ferrite-martensite interface are studied and the effect of martensite carbon content on these interatomic potentials is investigated. The equations developed here for the ferrite-martensite interface, combined with our earlier work on martensite cracking [16] will allow us to identify the dominant mechanism for failure initiation in DP steels as a function of martensite carbon content. This will be useful in the design of DP steels, and their composition, for industrial application.

Due to the very small ratio of carbon to iron atoms in martensite, the inclusion of explicit carbon atoms in martensite requires a very large super cell containing hundreds of Fe atoms with a few carbon atoms, which makes the DFT calculations very expensive. Nevertheless, we believe that the structural effect of trace amounts of a heteroatom in a crystalline material is reflected in the lattice constant variation of the host crystal structure, and therefore, the presence of heteroatom can be implicitly modeled if the relationship between the lattice constant and the concentration of heteroatom is known. However, it is noteworthy that in the implicit model, it is assumed that the dominant effect of the solute is its homogeneous changes to the host lattice constant. This assumption is valid as long as the heteroatom is uniformly distributed throughout the host crystal. Therefore, in our application of the implicit model, the validity of this assumption is dependent upon uniform distribution of carbon atoms in martensite. However, if the carbon segregates to the ferrite-martensite interface, the local concentration of carbon at the boundaries becomes greater than the bulk concentration. This phenomenon, which is also known as the “solute drag effect” [29], may influence the local boundary structure and electronic state at the interface. The solute drag effect has been previously observed in the segregation of Carbon,

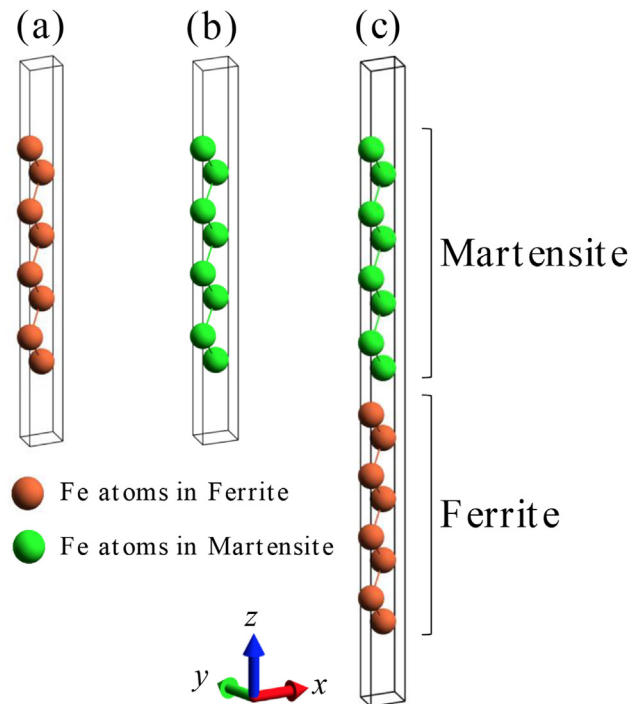


Fig. 2. Geometry of the a) ferrite, b) martensite and c) interface unit cells used in DFT calculation. The orange and green atoms represent the iron atoms in ferrite and martensite structures, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 1
Calculated bulk and surface parameters of α -Fe compared to the available experimental measurements [41,53,54].

Parameter	Calculated	Experimental	% Deviation
Lattice constant (Å)	2.8694	2.8665 (Ref. [41])	+0.10%
Magnetic moment (μ_B /atom)	2.19	2.22 (Ref. [53])	−1.35%
Fe (110) surface energy (J/m ²)	2.71	2.48 (Ref. [54])	+9.27%

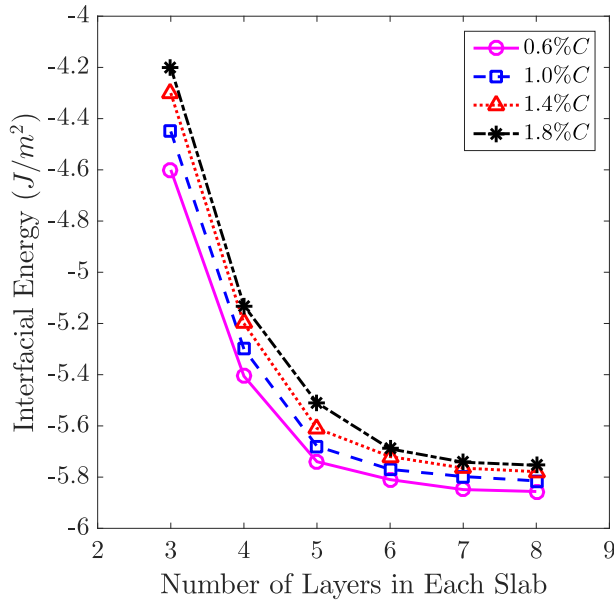


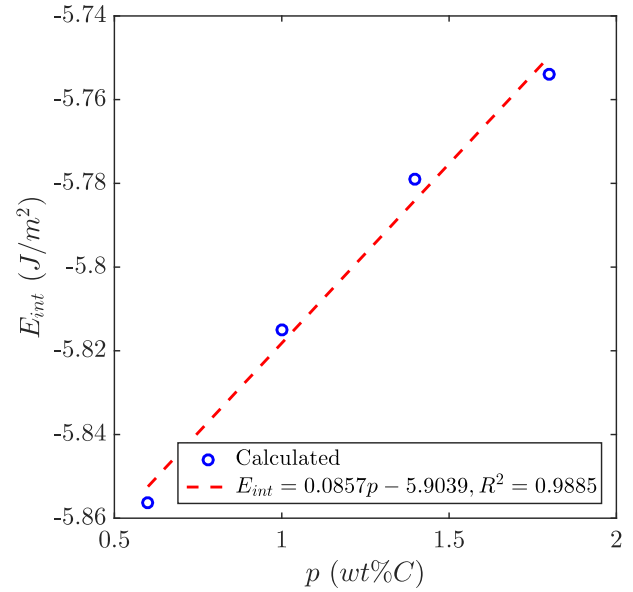
Fig. 3. The convergence of the interfacial energy with respect to the number of layers in each slab of the interface cell. Convergence is achieved at about 8 layers, after which the interfacial energy becomes almost independent of the slab thickness.

Molybdenum and Manganese to the ferrite-austenite boundaries in Fe-C-Mo and Fe-C-Mn-Si alloys [30–33]. Nevertheless, in this work we assume uniform distribution of carbon atoms throughout the martensite crystal structure, and therefore, the implicit model does not capture the potential effect of carbon segregation to the ferrite-martensite interface, due to the absence of explicit carbon atoms to account for the concentration gradient.

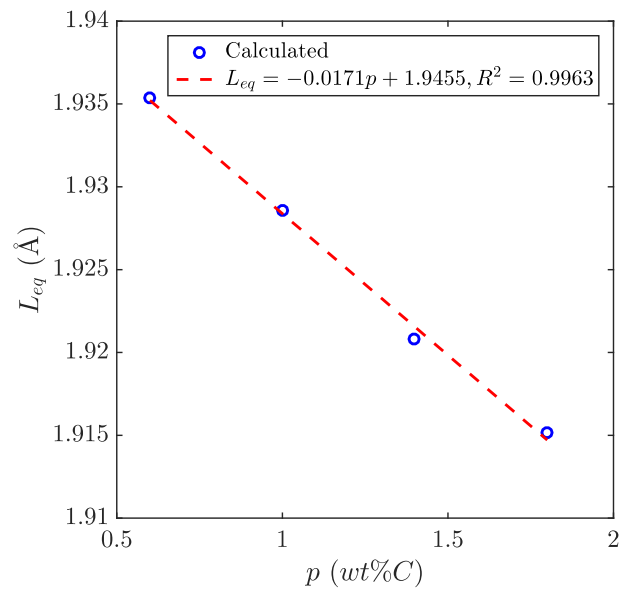
This implicit method is not limited to martensite and can be implemented in other materials such as n-type and p-type semiconductors with dopant impurities (group V and group IV elements) in an extremely pure intrinsic semiconductor such as silicon. For instance, the proportion of impurity to silicon in the degenerately doped silicon is on the order of parts per thousand [34]. This proportion may be reduced to parts per billion in very lightly doped silicon [35]. Therefore, the implicit method that utilizes lattice constant variations to account for such small amounts of impurities are potentially useful in studying the mechanical properties of these semiconductors in a computationally effective manner.

It should be noted that the implicit method might not be successful in studying the electronic properties of semiconductors using DFT since any change in the band gap is induced by the electronic structure of the impurities, which in this method do not explicitly exist in the crystal structure. In an extensive study, Zhao et al. [36] investigated the mechanism of insulator-to-metal transition of sulfur-doped silicon using expensive DFT calculations on unit cells consisting of up to 512 atoms since the sulfur concentration was explicitly varied by changing the ratio of silicon to sulfur atoms. In this study, they also reported the deviation of lattice constant and cell volume of sulfur-doped silicon compared to pure silicon [36], which can be useful in studying the mechanical properties of sulfur-doped silicon in a computationally inexpensive set of calculations using the implicit method.

In addition to the abovementioned assumptions, in the current study we have not considered any anisotropy or defect in the ferrite and martensite crystal structures. Therefore, due to the perfect crystal structures, the calculated interfacial energies are an upper bound for the actual values. While the inclusion of anisotropy and



(a)



(b)

Fig. 4. The variation of a) ferrite-martensite interfacial energy and b) equilibrium interfacial distance as a function of martensite carbon content. The corresponding linear fitted expressions are shown on each graph.

defects in the crystal structures are beyond the scope of the current study, future works will include these modifications to improve the accuracy of the model and provide a more realistic understanding of the ferrite-martensite interfacial properties.

2. Computational methodology

The main goal of the present study is to investigate the effect of martensite carbon content on the ferrite-martensite interfacial energy. It has been shown that both ferrite and martensite in the low carbon range up to 0.6 wt percent have a body centered cubic

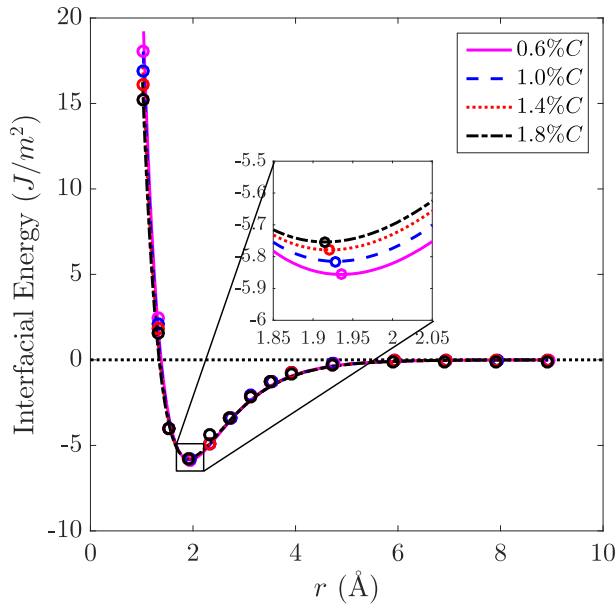


Fig. 5. The fitted Morse interatomic potentials between the atoms in the ferrite-martensite interface as functions of the separation (r) of the interfacial atoms for four different martensite carbon contents. The circle markers indicate the interfacial energy data points computed from ab initio calculations by varying the interfacial distance from 1 Å to 9 Å.

(BCC) structure [37]. However, it is known that the structure of high-carbon martensite changes suddenly to a body centered tetragonal (BCT) structure above 0.6 wt% carbon [38]. Fig. 1 shows the variation of the lattice parameters (a and c) of martensite with respect to its carbon content, which was established by Kurdjumov and Kaminsky [39,40]. This variation can be quantitatively described in the form of Eqs. (1a) and (1b):

$$a = a_0 - \beta p \quad (1a)$$

$$c = a_0 + \alpha p \quad (1b)$$

where p is the martensite carbon content in weight percent, a_0 is the lattice constant of α -Fe and is equal to 2.8665 Å [41], α and β are the slopes of the linear regressions and are equal to 0.116 ± 0.002 and 0.013 ± 0.002 Å/%C, respectively [40]. To investigate the effect of martensite carbon content on the ferrite-martensite interfacial energy, here we will vary the weight percent of carbon implicitly from 0.6 to 1.8 wt % by modifying the lattice constant of the BCT structure of martensite according to Eqs. (1a) and (1b). The choice of 1.8 wt% as an upper limit was made since according to the Fe-C phase diagram, the carbon content of austenite does not exceed 2.1 wt% in steel. Therefore, assuming complete austenite-to-martensite phase transformation during quenching, the concentration of carbon in martensite will be less

than 2.1 wt%.

First-principal density functional theory calculations are here utilized to determine the interfacial energy between the (110) surfaces of ferrite and martensite, which enables us to obtain the equilibrium interfacial distance as well. Spin polarized Kohn-Sham density functional theory [42] calculations were carried out using Quantum Espresso software package [43], a plane-wave [44] pseudopotential [45] code. The generalized gradient approximation was adopted to account for exchange correlation effects and an effective Hubbard $U_{\text{eff}} = 2.1$ eV was introduced within the GGA + U correction method [46] to remove the self interaction errors caused by the intra-atomic d- or f-interactions by introducing the effective onsite Coulomb interaction (U) term [47]. The obtained value for U is consistent with the calculated value for bcc iron in a study by Cococcioni et al. [48]. We employed the functional of Perdew, Burke and Ernzerhof (PBE) [49], which is suitable for describing metallic properties [50–52]. The core electrons are treated by projector augmented wave (PAW) pseudopotentials as applied in Quantum Espresso with a cut-off energy of 1100 eV obtained from a cut-off energy convergence test. The Brillouin zone integration for α -Fe bulk calculation has been performed on a $35 \times 35 \times 35$ k-point grid. In order to ensure the reliability of the results, the calculated α -Fe bulk and surface parameters are compared to the experimental measurements in Table 1.

The abovementioned validated pseudopotential and optimized lattice constants were utilized to create the initial geometry. As shown in Fig. 2(a) and (b), the pure structures of both ferrite and martensite were modeled by an 8-layer slab in a 1×1 geometry and a 6 Å vacuum space on the top and bottom sides of the slab using a $10 \times 10 \times 1$ k-point grid. The interface cell is modeled by a 16-layer slab containing 8 layers of ferrite and 8 layers of martensite vertically attached to each other as demonstrated in Fig. 2(c) using a similar 6 Å vacuum space on the top and bottom sides of the interface cell. All atoms were allowed to fully relax in all directions to minimize the stress on the interfacial atoms and optimize the interfacial energy. This procedure is performed for different martensite structures that correspond to the variation in carbon content from 0.6 to 1.8 wt % in 0.4% intervals. The relaxations have been performed until the forces were smaller than 0.005 eV/Å and the change in the total energy was smaller than 0.0003 eV.

Since the presence of the surfaces may affect the electronic state at the interface, the slabs need to be thick enough to minimize this effect. Therefore, the 8 layer slab for each phase (16 layers in total) was chosen based on a convergence test for the interfacial energy with respect to the number of layers in each slab. The convergence test was performed for all carbon contents (0.6–1.8 wt%) to ensure the independency of the obtained slab thickness from martensite carbon content. As shown in Fig. 3, the convergence of the ferrite-martensite interfacial energy is achieved at about 8 layers, after which the interfacial energy becomes almost independent of the slab thickness.

As shown in Eq. (2), the interfacial energy, E_{int} , is calculated by subtracting the total energy of pure ferrite ($E_{\text{ferrite}}^{\text{slab}}$) and martensite ($E_{\text{martensite}}^{\text{slab}}$) from the total energy of the interface cell ($E_{\text{int}}^{\text{slab}}$):

$$E_{\text{int}} = E_{\text{int}}^{\text{slab}} - [E_{\text{ferrite}}^{\text{slab}} + E_{\text{martensite}}^{\text{slab}}] \quad (2)$$

In addition to the interfacial energy calculation, the interatomic potentials between the atoms in the ferrite-martensite interface are studied and the effect of martensite carbon content on these interatomic potentials is investigated. A similar interface cell as the one used for the interfacial energy calculations was used for this simulation with the interfacial distance manipulated by varying the size of vacuum space between vertically adjacent surface cells. However, in this case, the two atoms in the ferrite-martensite

Table 2

The parameters of the ferrite-martensite Morse potentials obtained by fitting Eq. (4) on the calculated potentials for four different martensite carbon contents.

Carbon content (wt%)	Morse parameters		
	$D_e(\text{J/m}^2)$	$a(\text{\AA}^{-1})$	$r_e(\text{\AA})$
0.6	5.856	1.246	1.935
1.0	5.815	1.230	1.929
1.4	5.779	1.218	1.921
1.8	5.754	1.204	1.915

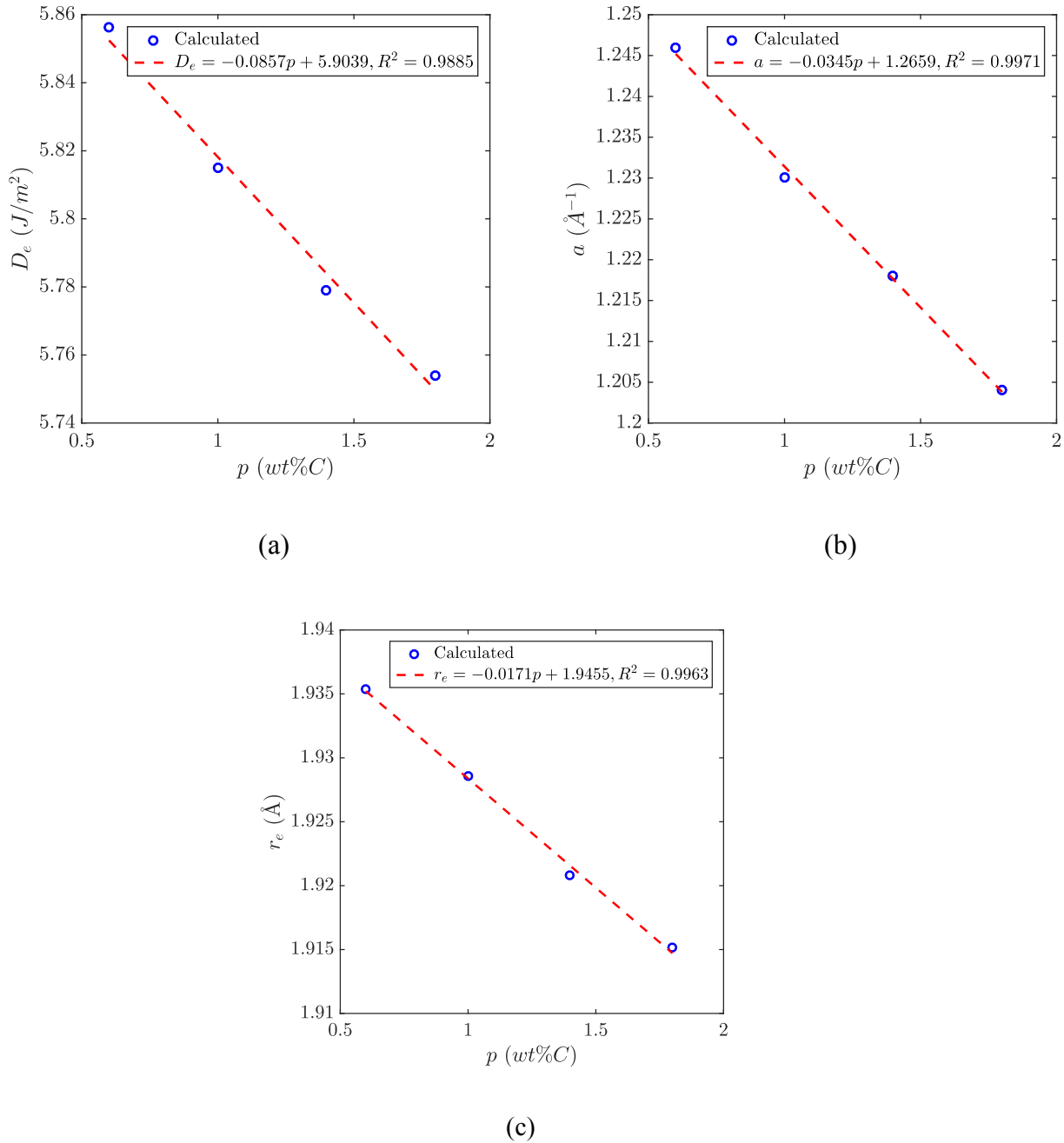


Fig. 6. Dependence on martensite carbon content of the following Morse parameters: a) well depth (D_e), b) potential width (a) and c) equilibrium interfacial distance (r_e). The corresponding linear fits, Eq. (5), are shown.

interface (one on each side) were allowed to relax only in the x and y directions while being fixed in z direction, in order to be able to manually control the interfacial distance. All other atoms were allowed to relax in all three directions. The interatomic distance in the z direction between the two interfacial atoms (interfacial distance) was varied from 1 Å to 9 Å and the total energy was calculated for each system. Similar to the interfacial energy calculations, the interatomic potentials were calculated by subtracting the total energy of pure ferrite ($E_{ferrite}^{slab}$) and martensite ($E_{martensite}^{slab}$) from the total energy of the interface cell (E_{int}^{slab}) as shown in Eq. (2).

3. Results and discussion

Fig. 4 shows that with increasing martensite carbon content, the magnitude of ferrite-martensite interfacial energy (E_{int}) decreases, as does the equilibrium distance between ferrite and martensite interfaces (L_{eq}). The empirical linear expressions fitted on the calculated data points shown in Eq. (3a) and (3b) can be used to predict the ferrite-martensite interfacial energy and interfacial distance, respectively, for a given martensite carbon content that lies within the studied range of 0.6–1.8 wt percent.

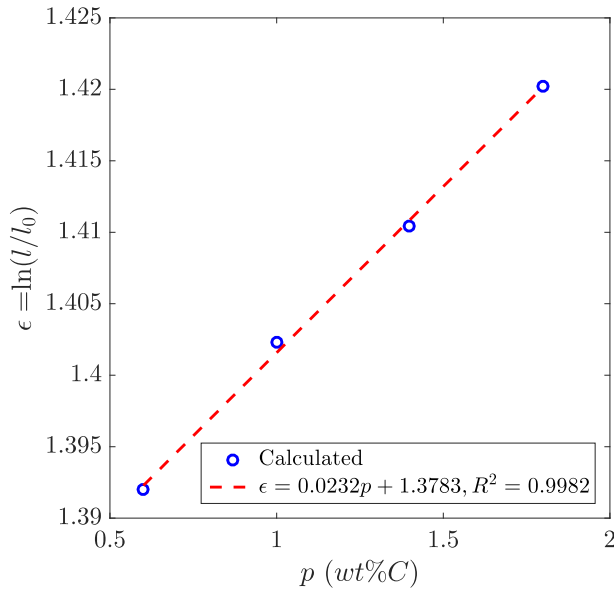


Fig. 7. The variation of the dissociation local strain at the ferrite-martensite interface against martensite carbon content along with the corresponding linear fit.

$$E_{int} = 0.0857 p - 5.9039 \quad (3a)$$

$$L_{eq} = -0.0171 p + 1.9455 \quad (3b)$$

In Eq. (3a) and (3b), E_{int} is the ferrite-martensite interfacial energy in J/m^2 , L_{eq} is the equilibrium interfacial distance between ferrite and martensite in Å, and p is the martensite carbon content in weight percent.

Fig. 5 shows the calculated interatomic potentials between the atoms in the ferrite-martensite interface for four different martensite carbon contents. As mentioned earlier, the data points were obtained by varying the interfacial distance from 1 Å to 9 Å and calculating the total energy of the system at each interfacial distance. The Morse interatomic potential in the form of Eq. (4) was used to fit the calculated data points [55]:

$$V(r) = D_e \left(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)} \right) \quad (4)$$

where $V(r)$ is the Morse potential, r is the interatomic distance in the z direction between the two interfacial atoms (interfacial distance), r_e is the equilibrium interfacial distance, D_e is the potential at its minimum i.e. $r = r_e$ (also known as the well depth) and a controls the width of the potential (the smaller a is, the larger the well). Note that in this form, $V(r)$ approaches zero at infinite r and equals $-D_e$ at its minimum. The Morse potential fits the computed potential well.

As shown in the magnified area of Fig. 5, the equilibrium interfacial distance and the magnitude of the interfacial energy decrease with increasing martensite carbon content. These trends are consistent with the results shown in Fig. 4, which are quantified in Eq. (3a) and (3b). The parameters of the ferrite-martensite Morse potentials obtained based on the best fit of Eq. (4) on the calculated potentials are presented in Table 2 for four different martensite carbon contents.

Moreover, the variation of the obtained Morse parameters against the martensite carbon content is shown in Fig. 6. The empirical linear expressions shown in Eq. (5a)–(5c) fitted on the calculated Morse parameters for four martensite carbon contents

can be used to predict the ferrite-martensite interfacial potential curve, for a given martensite carbon content that lies within the studied range of 0.6–1.8 wt percent.

$$D_e = -0.0857 p + 5.9039 \quad (5a)$$

$$a = -0.0345 p + 1.2659 \quad (5b)$$

$$r_e = -0.0171 p + 1.9455 \quad (5c)$$

The dissociation local strain is defined as the maximum local strain at the ferrite-martensite interface beyond which the interface separates, i.e. the interfacial energy becomes effectively zero and does not change by further increasing the interfacial distance. Mathematically, we assume that interface separation occurs when the first derivative of interfacial potential with respect to interfacial distance is less than $0.01 J/m^2/\text{Å}$ in the non-equilibrium region. Fig. 7 shows the variation of the dissociation local strain, obtained using this criterion, with martensite carbon content. The results indicate that by increasing the martensite carbon content, the dissociation local strain increases. The linear fit shown in Eq. (6) can be used to predict the dissociation local strain at the ferrite-martensite interface for a given martensite carbon content that lies within the studied range of 0.6–1.8 wt percent:

$$\epsilon = 0.0232 p + 1.3783 \quad (6)$$

where ϵ is the dissociation local strain at the ferrite-martensite interface, and p is the martensite carbon content in weight percent.

4. Conclusions

Ferrite-martensite interfacial energies and equilibrium interfacial distances for a series of martensite carbon contents were calculated using first-principles atomistic simulations. Spin polarized Kohn-Sham density functional theory [42] calculations were performed using Quantum Espresso software package [43], a plane-wave [44] pseudopotential [45] code, within the generalized gradient approximation. The effect of carbon content on the ferrite-martensite interfacial energy was determined by implicitly varying the carbon concentration from 0.6 to 1.8 wt percent by modifying the lattice constant of BCT martensite according to the empirical expressions of Kurdjumov and Kaminsky [39].

The results show that by increasing the carbon content, the magnitude of the ferrite-martensite interfacial energy is decreased, and the equilibrium interfacial distance is reduced. In addition to interfacial energies, the Morse interatomic potentials [55] between the atoms in the ferrite-martensite interface were calculated for four different martensite carbon contents, and the variations of the Morse parameters with the martensite carbon content were fit to linear expressions. Moreover, the dissociation local strains calculated from the interatomic potentials indicate that separating ferrite-martensite interface requires a higher strain at the interface when the martensite carbon content is higher. The simple equations fitted to the calculated data points can be used to predict the ferrite-martensite interfacial energy, equilibrium interfacial distance, dissociation local strain at the interface, and the Morse parameters for a given martensite carbon content that lies within the studied range of 0.6–1.8 wt percent. The results presented in this work can be used to further investigate the effect of martensite carbon content on the mechanical properties of steels.

Conflict of interest

The authors declare no competing financial interest.

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