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



Ali Ramazani ^{a,*}, Saeed Kazemiabnavi ^{b,1}, Ronald Larson ^a

^a Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109, USA

^b Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI 48109, USA

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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

* Corresponding author.

E-mail address: ramazani@umich.edu (A. Ramazani).

¹ S. Kazemiabnavi and A. Ramazani contributed equally.

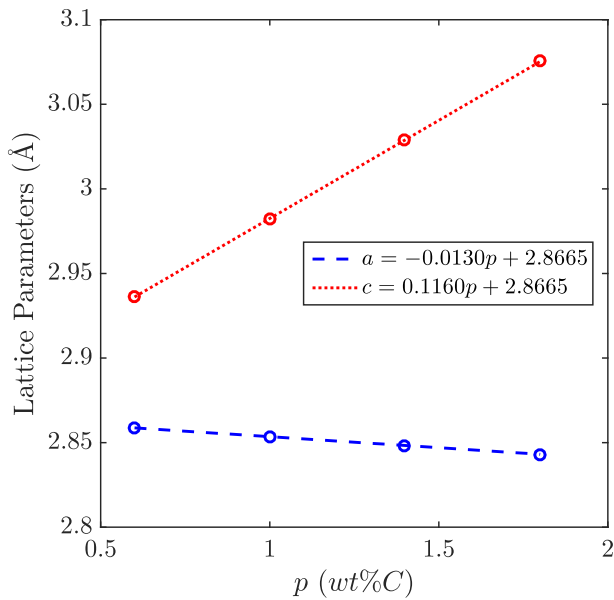


Fig. 1. The variation of the lattice parameters of high-carbon martensite ferrous with a body centered tetragonal (BCT) structure with respect to its carbon content. The linear regressions provided in Ref. [40] were used to obtain the lattice constants at the designated points [40].

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,

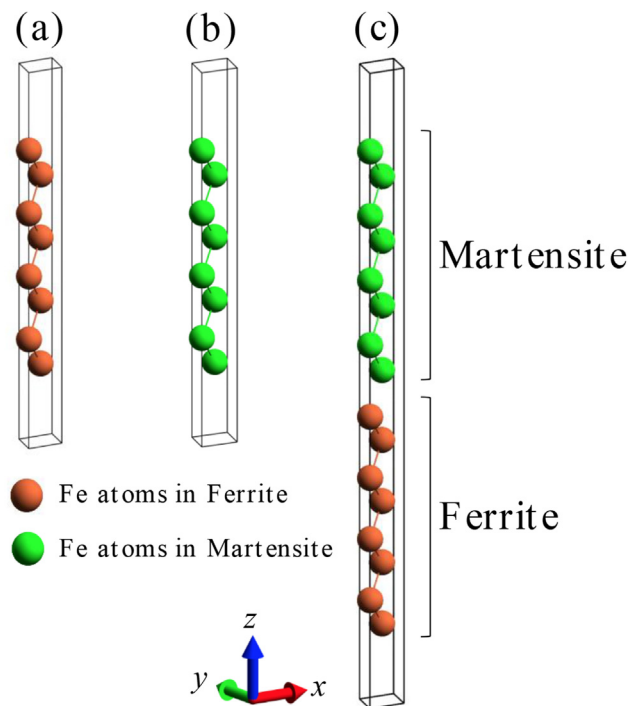


Fig. 2. Geometry of the a) ferrite, b) martensite and c) interface unit cells used in DFT calculation. The orange and green atoms represent the iron atoms in ferrite and martensite structures, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred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

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