ISSN (e): 2250 – 3005 || Vol, 04 || Issue, 12 || December – 2014 ||
International Journal of Computational Engineering Research (IJCER)

The Impact of Interstitial Carbon on Dislocation Motion in the alpha-Fe Lattice

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ABSTRACT:
The effect of the introduction of interstitial carbon into the α-Fe lattice on the behavior of dislocation cores is presented. The simulations carried out were based on an EAM formulation that generated stress cycles resulting from the movement of dislocations, caused by the rigid displacement of rows of atoms on one side of a slip plane. The "path of least resistance" (POLR) mechanism accounting for stress evolution at the dislocation core was applied to predict the Peierls stress. This paper presents the behavior of the edge and screw dislocations in the Fe-C lattice.

Keywords: *Embedded atom method; Body centered cubic; Dislocation cores; Peierls stress; Path of least resistance (POLR)*

I.INTRODUCTION

This study was conducted as part of a project to develop a multi-scale simulation platform utilizing atomic scale phenomena as input in a mechanistic plasticity model. This stage sought to model the behavior of dislocation cores in the Fe-C lattice. To characterize the behavior of the dislocation core, the interaction of dislocation core atoms was established using the embedded atom method (EAM). The behavior of dislocation cores in body centered cubic (BCC) iron and the effects of interstitial carbon on the evolution of the dislocations are reported.

The structure of the dislocation core has been used to predict the physical behavior of the dislocation in terms of motion and evolution, and to determine the strain energy and the Peierls stress at which these physical actions take place. Peierls stress calculations for BCC metals have been driven by the realization that their dislocation core effects contribute to a high Peierls stress [1]. However, most of the studies characterize the lattice resistance by the changes in the binding energy, and reports on computations and experiments determining the Peierls stress for Fe are few.

Several methods have been applied to predict the Peierls stress. The Peierls-Nabarro model [2,3] utilized inter-planar de-registry between rows of atoms to develop an analytical expression to predict the Peierls peak. This model did not account for the dislocation core structure and was initially confined to 2-dimensional geometry. Additionally, it was limited to a homogeneous system of atoms and did not account for variations in the inter-atomic interactions. A review of the evolution of this model was presented by Nabarro [4]. Lubarda and Markenscoff [5] proposed a variable core model to develop an analytical expression to predict the Peierls stress. Their model applied the shear stress of a distribution of infinitesimal dislocations to predict the energy of the whole stressed crystal between the stable equilibrium and the unstable states of the dislocation. This approach therefore did not apply the sinusoidal relationship between the shear stress and slip discontinuity along the slip plane as in the Peierls-Nabarro model [4].

Duesbery [6], Xu [7] and Wang et al. [8] presented the application of inter-atomic potentials in the computation of the core structure and the Peierls stress of dislocations. This method gave a more versatile approach to the modeling of varied spatial arrangements and elemental configurations. However, the method was limited to the suitability of the potentials used and the need to maintain a small atomic volume to accommodate computational limitations. Electronic structure calculations employing density functional theory based calculations were reported by Shimizu et al. [9,10]. This method was limited by the need to keep the simulation volume small, due computational constraints and the effects of boundary conditions on the electron field. This method has found application where a varied elemental configuration and non-equilibrium spatial arrangements are important.

In all these approaches, snapshots of various configurations of the evolving dislocation were considered. In contrast, Terentyev, Osetsky and Bacon [11] and Wang et al. [12] applied molecular dynamics to study the mobility of dislocations in BCC elements. In this approach, the application of dynamics allowed the spatial evolution of the lattice points to define the physical state of the material matrix, providing more realistic results in the computation.

Comparisons of the Peierls stress values determined by several different researchers [10,11,13,14] and the amplitude of the "path of least resistance" (POLR) stress [15] reveal some correlation between the two properties. The POLR value for the pure screw dislocation of 1.01 GPa [15] and symmetric screw dislocation of 1.883 GPa [15] compared well with density functional theory based calculations reported by Kaburaki [10] of a Peierls stress of 1.1 GPa for the screw dislocation in a stress driven computation with an initial symmetric screw dislocation configuration. However, Njoroge et al. [15] neglected to discuss the evolution of the configuration of the dislocation and it is unclear if the Peierls stress documented applies to the pure screw or the symmetric screw dislocation. These results [15] also suggested that the Peierls stress of the pure edge dislocation was higher than that of the pure screw dislocation. This inconsistency was explained by visualizing the edge dislocation motion as a multi-step translation of $[\bar{1}\,1\,1]$ and $[001]$ motions. The edge dislocation Peierls stress was therefore more closely related to the POLR value for the edge dislocation moving in the $[\bar{1}\,1\,1]$ direction of 1.578 GPa [15]. Similar inversion of relative Peierls stress values for the edge and screw dislocations were reported by Terentyev, Osetsky and Bacon [11]: 1.5 GPa for the edge dislocation and 1.4 GPa for the screw dislocation. They attributed this anomaly to the constriction of the edge dislocation core at the Peierls peak that inhibits dislocation motion.

Petukhov [16] reported a Peierls stress for a dislocation kink of 0.95 GPa. Available empirical findings on the dislocation kink [1] led to the conclusion that the edge dislocation component processes a greater mobility than the screw component. It may be inferred that the edge dislocation would have a Peierls stress in the order of 0.95 GPa. The POLR value of 1.578 GPa [15] for the edge dislocation moving in the $[\bar{1}\,1\,1]$ direction therefore compared much more favourably with the Peierls stress reported by Petukhov [16] and supported the assertion that the edge dislocation was more likely to move by a combination of $[\bar{1}\,1\,1]$ and $[001]$ motions. Terentyev, Osetsky and Bacon [11] reported a Peierls stress of 1.5 GPa at T=0K for a $\langle 100 \rangle$ edge dislocation in α-Fe. This result compared well with the POLR value for the $\langle \bar{1}12 \rangle$ edge dislocation moving in the $[\bar{1}\,1\,1]$ direction and further reinforced the assertion that the edge dislocation moved by a combination of $[\bar{1}\,1\,1]$ and $[001]$ motions [15]. Njoroge et al. [15] also showed an increase in the Peierls stress for the screw dislocation on the introduction of a symmetric dislocation core reconstruction. These findings therefore suggested that the screw components in dislocation kinks would contain appreciable sections of reconstruction defects, which would result in a higher POLR value for the screw component than the edge dislocation moving in the $[\bar{1}\,1\,1]$ direction. The POLR technique was therefore considered an acceptable approach in the estimation of the Peierls peak.

II.METHOD

Simulations in this work were carried out on computer code using the Fe-Fe potential developed by Mendelev et al. [17] in an embedded atom method formulation. This potential has been tested and found to stabilize the non-degenerate dislocation core sliding on $\{110\}$ glide planes, in agreement with experimental data for dislocation motion at low temperatures [13]. The formulation also applied the potential by Becquart et al. [18], which has been found to be suitable for modeling of a single element lattice with interstitial impurities. This combination of potentials was applied in this study of ferritic Fe-C solid solutions with low carbon concentrations.

Introduction of the initial distortion was achieved by the application of the distortion vector to atoms on one side of the slip plane. The distortion vector was selected such that together with the dislocation line, it defined the type of dislocation introduced. Dislocation flips were achieved by the application of displacement vectors to the core atoms, according to the definition of each type of dislocation flip. The resulting additional distortion was transferred to the dislocated lattice by a suitable algorithm. The carbon atoms were introduced at the octahedral interstitial sites at a frequency of one carbon atom in each BCC unit cell along the dislocation core.

Dislocation dynamics was achieved by rigidly displacing atoms on one side of the slip plane using atomic scale displacements. A uniform dislocation line displacement vector was applied. In this technique, no effort was made to attain equilibrium conditions, as these were considered unlikely in actual loading conditions. This work evaluated the stresses cycles and predicted the Peierls stress of the type of dislocation. The dislocation core stress components were calculated at lattice sites occupied by atoms adjacent to the slip plane. The simulations generated stress components σ_{ij} corresponding to the Cartesian coordinate system coincident with the edges of the BCC unit cell. Benchmarking of the simulation results was achieved by comparison with data generated by other researchers [10,13,14,16] using empirical and *ab initio* techniques.

III.RESULTS AND DISCUSSION

Simulations of the motion of the edge and screw dislocations were carried out and curves of the six independent stress components plotted in Figures 1 and 2. All dislocations generated cyclic stress variations for all stress components, differing in the pattern formed and the amplitude of individual curves. The cyclic behaviour is consistent with dislocation behaviour described in the Peierls-Nabarro model [19,20]. The positive and negative values were interpreted as tensile and compressive stresses respectively, and it was noted that the direct stress were negative for the Fe-C lattice.

1.1. Screw Dislocation

The stress curves for screw dislocation core in the Fe-C lattice are presented in Figure 1. The curves show an increase in stress component values of -21.9 GPa to -26.4 GPa, up from 5.41 GPa to -6.44 GPa in the carbon free lattice [15]. The introduction of interstitial carbon in the Fe lattice therefore resulted in a considerable increase in lattice resistance to dislocation motion. These results are in qualitative agreement with existing knowledge where carbon in the Fe lattice enhances yield strength. In addition, the introduction of interstitial carbon resulted in compressive stresses in the dislocation core as the dislocation moved through the lattice. This observation is consistent with the formation of matensite in the Fe-C lattice, which forms as a body centered tetragonal (BCT) structure above a concentration of 0.6% carbon by mass [21], and which is closely related to the BCC lattice adopted by the simulations.

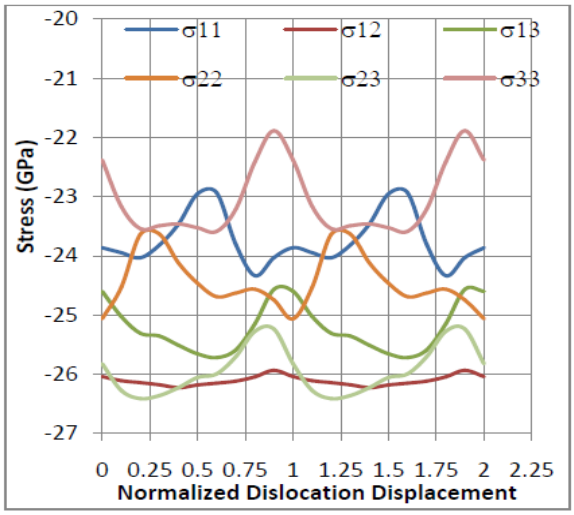

Fig. 1: Stress amplitude generated as a pure screw dislocation in the Fe-C lattice moves in the $[1\bar{1}1]$ direction.

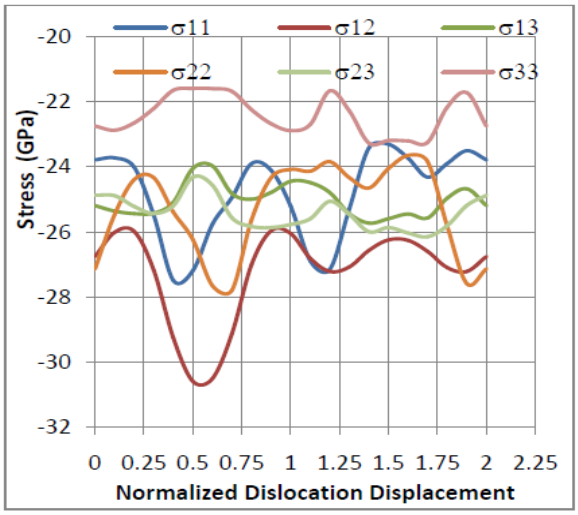

Fig. 2: Stress amplitude generated as a pure edge dislocation in the Fe-C lattice moves in the $[\bar{1}12]$ direction.

The curves in Figure 1 give a POLR value of 1.6 GPa. The directions generating the POLR correspond to σ_{33} and σ_{11} stress components, with σ_{33} providing the major contribution. It is also noteworthy that the direct stresses provide the POLR, as was the case in for the carbon-free lattice [15]. The amplitude of the POLR changed from 1.01 GPa [15] to 1.6 GPa as interstitial carbon was introduced. This is consistent with the expected strengthening of the lattice with introduction of interstitial carbon. The stress amplitude is of the same order of magnitude as the Peierls stress, and it is suggested that this parameter is more closely related to the Peierls stress than the absolute stress value of the stress cycle.

1.2.Edge Dislocation

The stress curves for edge dislocation core in the Fe-C lattice are shown in Figure 2. The POLR amplitude increased from 1.578 GPa for the edge dislocation moving in the $[\bar{1}11]$ direction [15] in a carbon-free lattice to 1.7 GPa in the Fe-C lattice. This increase in amplitude suggests that dislocation mobility decreased on the introduction of carbon into the lattice. This is consequent with empirical findings at the macro-scale which suggest that dislocation motion is inhibited by interstitial carbon atoms [22].

The pattern of the stress curves for the Fe-C lattice is similar to that observed for the carbon-free lattice. However, unlike the curves for the carbon-free lattice, the intersections of stress component curves were reduced, implying a reduction in the number of degrees of freedom of motion for this dislocation. Consequently, it was concluded that the edge dislocation motion in the Fe-C lattice should experience a reduction in the ability of dislocation core atoms to "peel" around the core, and this would result in a lower mobility of this dislocation. This inference is consistent with the relatively brittle nature of the Fe-C lattice.

1.3.The Peierls Stress For BCC Lattice Structures

A summary of the active stresses simulated by the POLR for the Fe-C lattice is shown in Table 1. The results reveal an increase in the stress amplitude for the screw and the edge dislocations consistent with expectations. Clouret et al. [23] demonstrated that the binding energy of the carbon atom to dislocation core sites was higher for the edge dislocation than the screw dislocation. A consequence of this observation was that carbon forming Cottrell atmospheres would result in more effective pinning of the edge dislocation core, and hence a higher Peierls stress [23]. This was consistent with the current results where the edge dislocation presented a higher POLR value than the screw dislocation.

Table 1: The stress range for the POLR for the Fe-C lattices

Dislocation Type	Stress Range (GPa)		Stress Amplitude (GPa) - POLR	Peierls stress (GPa)
	Lower	Upper		
Symmetric screw	-22.3	-24.0	1.7	-
Anti-symmetric screw	-22.7	-26.8	4.1	-
Pure screw	-21.9	-23.5	1.6	1.2 - 1.8 [11,13] 1.3 - 1.8 [14] 1.1 [10]
70.53° screw	-21.6	-23.2	1.6	-
35.26° screw	-21.5	-23.4	1.9	-
Pure edge	-21.6	-23.3	1.7	1.5 [11]

IV. CONCLUSIONS

It is concluded that the path of least resistance (POLR) stress is related to the Peierls stress for the Fe-C lattice. It is also concluded that the Peierls stress is attributed to the contribution of dislocation core direct stress components, and that the variation of the POLR stress between the different dislocation types is not significant in the Fe-C lattice. It is noted that data on the stress tensor components in Fe-C lattice as dislocations move through the lattice have not been presented elsewhere, to the best of the authors' knowledge.

ACKNOWLEDGEMENTS

This research has been supported by the African Materials Science and Engineering Network (AMSEN) funded by the Carnegie Corporation of New York. This support is greatly appreciated.

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