Role of disconnections in mobility of the austenite-ferrite inter-phase boundary in Fe

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Abstract

Austenite (γ-Fe, face centered cubic (FCC)) to ferrite (α-Fe, body centered cubic (BCC)) phase transformation in steel is of great significance from the point of view of industrial applications. In this work, using classical molecular dynamics simulations, we study the atomistic mechanisms involved during the nucleation and growth of the ferrite phase embedded in an austenite phase. We find that the disconnections present at the inter-phase boundary can act as the nucleation centers for the ferrite phase. Relatively small interface velocities (1.19 - 4.67 m/s) confirm a phase change via massive transformation mechanism. Boundary mobilities obtained in a temperature range of 1000 to 1400 K show an Arrhenius behavior, with activation energies ranging from 30 - 40 kJ/mol.

I. INTRODUCTION

During the process of iron and steel making, as molten Fe is cooled, first it solidifies to δ (BCC) allotrope of iron at a temperature of 1811 K. This is followed by solid-solid phase transformations, initially from δ-Fe to γ-Fe (FCC) at 1667 K and finally from γ-Fe to α-Fe (BCC) at 1185 K. The latter is very important, because the microstructure and mechanical properties of Fe-alloys are governed by the amount of austenite (γ-Fe) and ferrite (α-Fe) present after the transition. Being a very complex process, governed by several extrinsic (composition, rate of cooling etc.) and intrinsic (nucleation, inter-phase and grain boundary mobility, relative orientation of the two phases etc.) factors, the atomistic mechanisms involved during the phase transition are not clearly understood yet. Based on several experimental studies, it has been established that the nature of the transition is either martensitic or massive.1,2 The former is a diffusion-less transformation, which takes place via a coordinated movement of atoms by a distance less than the interatomic spacing. On the other hand, massive transformation occurs via nucleation and growth of the ferrite phase at the expense of the austenite phase, driven by Gibbs free energy change.

In order to describe the kinetics of the γ-α transformation, mainly two types of models have been proposed in the literature: diffusion controlled growth model3 and interface controlled growth model.4 In reality, transformations are mixed in nature, starting as an interface controlled process and following the initial stages of nucleation and growth, a relatively slow diffusion controlled process takes over.5,6 The interface controlled phase transformation is characterized in terms of intrinsic mobility of the inter-phase boundary and values ranging from 10^{-6} to 10^{-9} m·mol/(J·s) have so far been reported in the literature.2,6,7 Boundary mobilities are also known to show an Arrhenius behavior, with activation energy reported to be ≈ 140 kJ/mol.2,6,7

Since the nucleation and growth of the ferrite phase starts at the γ-α inter-phase boundary, orientations of the two phases at the interface play a crucial role in transformation. Several orientation relationships (OR) between the FCC and BCC phase have so far been proposed in the literature. This includes Bain,8 Nishiyama-Wasserman (NW),9 Kurdjumov-Sachs (KS),10 Greninger-Troiano (GT),11 and Pitsch.12 Other than the Bain and Pitsch, interface is formed between the two closest packed planes of the two phases, i.e., (111)FCC || (110)BCC. Pitsch OR is exactly opposite to this, with (111)BCC || (110)FCC. In case of Bain OR, interface is formed between the (001) plane of both the phases. Among all the ORs, NW and KS are more often reported in case of iron and steel.13

Because of its length and time scale, interface controlled γ-α phase transformation can be investigated by atomistic calculations14–17 and several studies related to massive and martensitic transformations based on classical molecular dynamics simulations have been reported so far.18–25 During martensitic transformations, interface velocities are found to be very high, ranging between 200-700 m/s in case of Bain and KS ORs at different temperatures.20 On the other hand, much smaller interface velocities (0.7-3.4 m/s) are obtained in case of massive transformation, as reported for a γ − α interface of NW type.21,22 A comparison between the NW and KS ORs reveals planar and needle like growth of the ferrite phase taking place at the respective interfaces, the former being ten times slower than the latter.23 Bi-directional transformations are also reported in case of NW orientation, with significant difference of interface velocity between the γ − α (24 m/s) phase change and vice versa (240 m/s).24

Interestingly, in many of the computational studies mentioned above, some kind of defect (like a free surface, stacking faults, twin boundaries, steps present at the γ − α interface etc.) is present in the initial structure, which assists the phase transformation. Motivated by this, we focus on a particular type of defect, known as disconnections. This a type of interfacial defect having both dislocation and step-like character.26–28 Disconnections are reported to be observed at the inter-phase boundaries of several ferrous and non-ferrous materials.29–33 They are also reported to play important role during the phase transformation.27,28,34–36 In this paper we investigate role of disconnections during the austenite to ferrite...
transformation in pure-Fe, using classical molecular dynamics simulations. Our study clearly shows that the nucleation of the $\alpha$-Fe phase starts at the disconnections located at the austenite-ferrite interface, which moves like a vertical wall to complete the transformation. We also calculate the velocity and mobility of the $\alpha - \gamma$ interface and the values suggest a massive transformation from $\gamma$-Fe to $\alpha$-Fe.

The paper is organized as follows: in Sec. II we discuss the simulation details, which include A) a discussion on interatomic potential, B) calculation of driving force for the phase transformation, C) crystallographic description of the simulation box and D) calculation of interface velocity and mobility. This is followed by a detailed discussion of the main results obtained in this work in Sec. III and the paper is concluded in Sec. IV.

II. SIMULATION DETAILS

A. Interatomic Potential

All the calculations are performed using classical molecular dynamics (MD) simulations, as implemented in Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package. Interaction among metal atoms are well approximated by EAM (embedded atom method) potentials. In this work we use the empirical potential developed by Ackland et al. Using this potential, calculated values of lattice parameter, cohesive energy, vacancy formation energy and elastic constants are found to be in very good agreement with experimental data, as well as density functional theory (DFT) based predictions [see Table I]. However, there are two drawbacks of this potential; first, it overestimates the melting point [see Table I] and second, the BCC phase remains more stable than FCC up to the melting temperature. In reality, a BCC to FCC phase transition is observed at 1185 K in the experiments, which can not be captured by this empirical potential. Despite these limitations, Ackland potential has been used in numerous MD studies on Fe, including the FCC to BCC phase transition.

B. Driving Force for the Phase Transformation

It is well known that the driving force behind massive transformation is the reduction of the Gibbs free energy ($\Delta G_{\gamma \rightarrow \alpha}$) as Fe transforms from the austenite to the ferrite phase. In order to calculate $\Delta G_{\gamma \rightarrow \alpha}$, we first calculate $\Delta G_{L-S}$, the free energy difference between the liquid (L) and solid (S) phase using the Gibbs-Helmholtz equation,

$$\frac{\Delta G_{L-S}}{T} = \int_{T}^{T_m} \frac{H^S(T) - H^L(T)}{T^2} dT, \quad (1)$$

where $H$ is the enthalpy, which is a function of temperature $T$ and $T_m$ is the melting point. The calculation is carried out separately for both $\alpha$ and $\gamma$ solid phases from 1800 to 2200 K at an interval of 100 K [see Fig. 1].

| Property | Experiment | Ackland et al. (1997) |
|----------|------------|-----------------------|
| $a$ ($\text{Å}$), BCC at $T=0$ K | 2.855$^a$ | 2.866 |
| $a$ ($\text{Å}$), FCC at $T=0$ K | 3.658$^a$ | 3.680 |
| $T_m$(K) | 1812$^a$ | 2358 |
| $E_{coh}$ (ev/atom) | -4.316$^a$ | -4.316 |
| $E_f$(ev/atom) | 1.84$^a$ | 1.89 |
| C$_{11}$ (GPa) | 242.00$^b$ | 243.39 |
| C$_{12}$ (GPa) | 146.50$^b$ | 145.03 |
| C$_{44}$ (GPa) | 112.00$^b$ | 116.00 |

$^a$ Values taken from Mendelev et al.(2003)$^{41}$

$^b$ Values taken from Hirth and Lothe (1968)$^{42}$

| Temperature(K) | 1000 | 1200 | 1400 |
|----------------|------|------|------|
| $\Delta G_{\gamma \rightarrow \alpha}$ (ev/atom) | 0.0198 | 0.0183 | 0.0168 |
| $\Delta G_{\gamma \rightarrow \alpha}$ (kJ/mole) | 1.912 | 1.767 | 1.622 |

FIG. 1. Free energy difference between the liquid and solid phase ($\Delta G_{L-S}$) for both $\alpha$-Fe and $\gamma$-Fe. Free energy difference between the solid phases ($\Delta G_{\gamma \rightarrow \alpha}$) is calculated from the vertical difference between the two lines.
cooled) to get the potential energy, equal to the enthalpy of the liquid phase at a given temperature \( (H^L(T)) \). In order to estimate the melting point, we use the coexistence method (developed by Morris and Song) and \( T_m \) for the BCC and FCC phase are found to be 2358 K and 2237 K, respectively.

Calculated values of \( \Delta G_{L-S} \) are illustrated in Fig. 1, along with a linear fit of \( \Delta G_{L-S} \) as a function of temperature, as shown below:

- FCC: \( \Delta G_{L-S} = 6.495 \times 10^{-5}T - 0.1469 \),
- BCC: \( \Delta G_{L-S} = 7.245 \times 10^{-5}T - 0.1742 \).

Finally, the free energy difference between the solid phases \( (\Delta G_{\gamma-\alpha}) \) is obtained from the vertical difference between the two lines at any given temperature. The lines shown in Fig. 1 are extrapolated to get the value of \( \Delta G_{\gamma-\alpha} \) at lower temperature, lying in the range of 1000 K to 1400 K. As reported in Table II, in the temperature range of 1000 to 1400 K, \( \Delta G_{\gamma-\alpha} \) values predicted by EAM potential lie in the range of 1.912 to 1.622 kJ/mole. Although the value dips a bit with increasing temperature, the system is still far from the ferrite to austenite transformation even at 1400 K. This is a well known drawback of the Ackland potential, which prefers ferrite over the austenite phase all the way to the melting temperature. Comparing with the experimental results, it is found that the numerical values of \( \Delta G_{\gamma-\alpha} \) obtained from the Ackland potential in this study [see Table II] are equivalent to the actual free energy difference at a temperature range of roughly 700-750 K. Thus, driving force applied in this study is not completely out of range.

C. Simulation Box Details

Since our goal is to study the FCC to BCC phase transition, we must have both the phases present in the beginning. For this purpose, initially we create a BCC and a FCC box separately. The crystallographic directions parallel to the box edges and sizes of the boxes in terms of number of atomic planes present along a particular direction is reported in Table III. The cross section \( (yz \text{ plane}) \) of both the boxes are adjusted such that the interface strain remains less than 1% after we join the two phases at a later stage. First, both the boxes are equilibrated separately for 2 ns using a NVT ensemble to bring all the atoms in thermal equilibrium. This is followed by a 6 ns run using a NPxT ensemble for the purpose of volume equilibration, without altering the interface area.

After equilibration, boxes are joined in a sequence of BCC-FCC-BCC, making a sandwich like structure [see Fig. 2]. After joining the two phases, the simulations box remains fully periodic, having no free surface and there are two BCC-FCC interfaces within the box. Interface is formed parallel to the \( yz \) plane and the growth direction (of the BCC phase) is perpendicular to the interface (along the \( x \) axis). Since NW is one of the most commonly observed orientation relationship between the BCC and FCC phase, we select this among various possibilities (as mentioned in Sec. I) to create the austenite-ferrite interface in this work. NW is a semi-coherent interface between the closest packed planes of BCC and FCC phase, described as \( (110)_{BCC} \parallel (111)_{FCC} \) and \( [001]_{BCC} \parallel [110]_{FCC} \). In case of ideal NW orientation
TABLE III. Crystallographic orientations parallel to the $x$, $y$, and $z$ direction of the simulation boxes used in this work.

| Phase | Direction | Orientation | Size (no. of atomic planes) | Tilt angle |
|-------|-----------|-------------|----------------------------|------------|
| BCC   | $x$       | [110]       | 16                         | -          |
|       | $y$       | [110]       | 42                         | -          |
|       | $z$       | [001]       | 54                         | -          |
| FCC   | $x$       | [111]       | 180                        | 0°         |
|       | $y$       | [112]       | 37                         | 0°         |
|       | $z$       | [110]       | 60                         | 0°         |
| FCC   | $x$       | [998]       | 180                        | 3.11°      |
|       | $y$       | [449]       | 37                         | 3.11°      |
|       | $z$       | [110]       | 60                         | 3.11°      |
| FCC   | $x$       | [779]       | 180                        | 4.04°      |
|       | $y$       | [337]       | 37                         | 4.04°      |
|       | $z$       | [110]       | 60                         | 4.04°      |
| FCC   | $x$       | [554]       | 180                        | 5.77°      |
|       | $y$       | [225]       | 37                         | 5.77°      |
|       | $z$       | [110]       | 60                         | 5.77°      |

After creating the simulation box with both the phases present in it [see Fig. 2(a)], we finally run the dynamics using a NP$_x$T ensemble until the FCC phase completely transforms into the BCC phase [see Fig. 3]. Depending on the temperature, it takes around 4 to 15 ns for the transformation to complete. The transformation can also be tracked by monitoring the change of potential energy, which continuously decreases as the fraction of BCC phase increases with time [see Fig. 4 and Fig. 5].

D. Interface Velocity

The speed ($v$) at which the austenite-ferrite interface moves can be estimated from the rate of change of potential energy ($\frac{dE}{dt}$) during the transformation [see Fig. 4] using the following equation:

$$v = \frac{\Omega}{2aL} \frac{dE}{dt},$$

where $a$ is the area of interface connecting the two phases, $L$ is the latent heat of solid-solid phase transformation (enthalpy difference per atom between the $\alpha$ and $\gamma$ Fe) and $\Omega$ is the volume per atom in the FCC phase. The factor 2 in the denominator takes into account the two FCC-BCC interfaces present in the simulation box. The velocity ($\vec{v}$) at which the austenite-ferrite interface moves is proportional to the driving force for the phase transition ($\Delta G_{\gamma-\alpha}$),

$$\vec{v} = \vec{M} \Delta G_{\gamma-\alpha}, \tag{3}$$

where $\vec{M}$ is the interface mobility. Using the calculated values of $v$ and $\Delta G_m$, we further estimate the numerical value of interface mobility, which is related to the activation energy required for one atom present in the FCC phase to cross the inter-phase boundary due to thermal fluctuations and get attached to the BCC phase. The activation energy ($Q$) is calculated from the following equation

$$\vec{M} = \vec{M}_0 \exp \left( -\frac{Q}{RT} \right), \tag{4}$$

where $R$ is the universal gas constant.

III. RESULTS AND DISCUSSIONS

Among the four different BCC-FCC interfaces [see Fig. 2 and Table III], no phase transformation is observed in case of ideal NW OR. However, when the FCC region is tilted with respect to the ideal NW OR, FCC to BCC phase transformation is indeed observed. As shown in Fig. 3, nucleation and growth of the BCC phase (blue) starts from both end of the simulation box and the FCC phase (green) is transformed in due course of time, ultimately converting the entire box to BCC phase. Lack of phase transformation in case of ideal NW type interface is probably due to the absence of any defect sites, required for nucleation of the BCC phase. On the other hand, in case of other orientations (tilted with respect
Tracking the $\gamma - \alpha$ phase transformation can simply be done by monitoring the potential energy of the system as a function of time. Since $\gamma$ has higher free energy than that of $\alpha$ [see Fig. 1], the potential energy of the system is going to decrease as the former is transformed into the latter phase. This is shown in Fig. 4 (a)-(c) for three differently oriented FCC phases at three different temperatures. For a given orientation, the phase transformation is faster at higher temperature [see Fig. 4 (a)-(c)]. This is because activation energy required for an atom in the $\gamma$ phase to detach from its parent FCC lattice, cross the interface and attach to the BCC lattice of the $\alpha$ phase is provided by thermal fluctuations and this process is facilitated at higher temperature.

It would also be interesting to compare the rate of transformation among three different orientations of the FCC phase at a given temperature. Change of potential energy as a function of time during the transformation is plotted in Fig. 5 (a), (b) and (c) for 1000, 1200 and 1400 K, respectively. Clearly, higher the tilt of the FCC phase with respect to the ideal NW OR, faster is the rate of transformation to the BCC phase. As already shown in Fig 2 (c)-(e), higher tilt angle with respect to the ideal NW OR results more steps or disconnections in the FCC side of the interface. Thus, these steps must be playing some important roles during the phase transformation to the ideal NW OR) steps or disconnections are present at the interface [see Fig. 1], which act as possible sites of heterogeneous nucleation of the BCC phase. This is going to be discussed in detail later in this section.

FIG. 4. Change of potential energy as the FCC transforms to the BCC phase at 1000, 1200 and 1400 K. The FCC phase is rotated by (a) 5.77°, (b) 4.04° and (c) 3.11° from the ideal NW OR. Evidently, the transformation takes lesser time at higher temperature.

FIG. 5. Change of potential energy as the FCC transforms to the BCC phase at (a) 1000, (b) 1200 and (c) 1400 K. A comparison is shown among three orientations of FCC phase with respect to the ideal NW OR; 998 (5.77°), 776 (4.04°), 554 (3.11°). Clearly, the transformation takes lesser time at higher angle.
TABLE IV. Interface velocities calculated (using Eq. 2) at different orientations and temperatures. These numbers are calculated by taking average of the values obtained from eight independent simulations starting with different initial velocities for each of the temperature and orientation. The unit of interface velocity is m/s.

| Orientation | T=1000 K | T=1200 K | T=1400 K |
|-------------|----------|----------|----------|
| 5.77°       | 1.98±0.29 | 3.24±0.28 | 4.67±0.21 |
| 4.04°       | 1.46±0.09 | 2.59±0.19 | 4.25±0.15 |
| 3.11°       | 1.19±0.15 | 2.28±0.21 | 4.11±0.23 |

process. Considering the fact that no transformation is observed in case of atomically flat ideal NW OR, as well as phase transition rate being enhanced with increasing number of steps at the interface, it appears that the steps or disconnections act as nucleation centers for the BCC phase. This hypothesis is further confirmed by taking snapshots of the simulation box at various time steps during the transformation. Three such configurations, one each for every orientation considered in this paper, are shown in Fig. 6 (a)-(c), where only the BCC phase is illustrated for the sake of visual clarity. Comparing with Fig. 2(c)-(e), we conclude that depending on the number of steps or disconnections present at the interface [see Fig. 2(c)-(e)], there are as many nucleation centers for the ferrite phase.

After uncovering the atomistic mechanism of austenite to ferrite phase transformation, we now estimate the speed at which the austenite-ferrite interfaces move during the transition. Interface velocity is calculated using Eq. 2, where \( \frac{dE}{dt} \) is taken to be the slope obtained from a linear fit of the potential energy profiles during the transformation [see Fig. 4 and Fig. 5]. Calculated values of interface velocity (reported in Table IV) lie in the range of 1.19 to 4.67 m/s, depending on the temperature and orientation of the austenite phase. Note that, interface velocities reported in Table IV are calculated by averaging the values obtained from eight independent simulations starting with different initial velocities for each of the temperature and orientation. Comparing with the values reported in the literature,\,^{20,21} interface velocities obtained in the present work are significantly lesser than that of martensitic transformation, but similar to that of massive transformation. This further confirms the transformation in the present work to be massive in nature. As expected, interface velocity for any particular orientation increases with temperature because higher thermal energy helps the atoms to cross over from the austenite to the ferrite site. Interestingly, at a given temperature, interface velocity increases as the austenite phase is tilted further away from the ideal NW OR. This is possibly because, with increasing number of the nucleation sites in the form of steps or disconnections, ferrite phase nucleates more rapidly at the interface, leading to faster movement of the boundary at higher tilt angles.

Finally, we estimate the mobility of the interface during the austenite-ferrite transformation using Eq. 3. Driving force and interface velocity data are taken from

FIG. 6. Nucleation of the ferrite phase at the interface. Atoms belonging to the ferrite (BCC) phase are only shown in this figure, while the snapshot is taken at some intermediate time step during the transformation. With respect to the ideal NW OR, the austenite phase in this particular case is tilted by (a) 5.77°, (b) 4.04° and (c) 3.11°. Depending on the number of steps or disconnections present at the interface [see Fig. 2(c)-(e)], there are as many nucleation centers for the ferrite phase.

FIG. 7. Interface mobility plotted as a function of inverse of the absolute temperature for different orientations of the austenite phase with respect to the ideal NW OR. The slopes of the fitted lines give the value of activation energies [see Eq. 4].

TABLE V. Interface mobilities calculated (using Eq. 3) at different orientations and temperatures. Similar to Table IV, data from eight independent calculations are averaged to get the values of mobility for each of the temperature and orientation. The unit of mobility is \( 10^{-3} \) m-mol/(J-s).

| Orientation | T=1000K | T=1200K | T=1400K |
|-------------|---------|---------|---------|
| 5.77°       | -1.0±0.15 | 1.8±0.16 | 2.9±0.13 |
| 4.04°       | 0.8±0.05 | 1.5±0.11 | 2.6±0.09 |
| 3.11°       | 0.6±0.08 | 1.3±0.12 | 2.5±0.14 |
Table II and Table IV, respectively. Calculated values of mobility are reported in Table V. Since interface velocity increases and $\Delta G_{\gamma - \alpha}$ decreases with temperature, mobility for a given interface orientation enhances with increasing value of $T$. Interestingly, at a particular temperature, mobility increases with the angle of tilt of the austenite phase with respect to the ideal NW OR [see Table V]. This is directly related to the enhancement of the interface velocity with the tilt angle at any particular temperature, as reported in Table IV. Activation energy $Q$ [see Eq. 4] is estimated from the slope of the ln $M$ vs. $\frac{1}{T}$ line, as illustrated in Fig. 7 for all three different orientations of the austenite phase. Clearly, $Q$ decreases with increasing tilt angle from the ideal NW OR. The numerical values of the activation energies are found to be 29.62, 35.60 and 40.63 kJ/mol, when the austenite phase is tilted by 5.77, 4.04 and 3.11°, respectively.

Comparing with experimental data, calculated values of activation energies are found to be 3 to 4 times lower in our simulations, which means faster transition from the austenite to the ferrite phase. There can be several reasons behind this anomaly. Firstly, we simulate pure Fe, while most of the experiments are for Fe-C-X (where X can be Mn, Ni etc.) type of alloys and alloying elements can slow down the rate of transformation. Secondly, in our study $\alpha - \alpha$ and $\gamma - \gamma$ grain boundaries are absent. In reality, there exist a network of grain boundaries, which can hinder the mobility of $\alpha - \gamma$ inter-phase boundary. Thirdly, since we are using the Ackland potential, the driving force for the phase transition is in the higher side. In reality, driving force is very small close to the $\alpha - \gamma$ transition temperature (1185 K), which can not be captured by this particular potential. However, the atomistic mechanism of nucleation and growth of the ferrite at its interface with the austenite phase is unlikely to be dependent on the choice of the empirical potential. We believe that our results are correct in this regard.

IV. SUMMARY AND CONCLUSIONS

In conclusion, we present a detailed analysis of the roles played by disconnections, which appear as steps at the $\alpha - \gamma$ inter-phase boundary, during the austenite to ferrite phase transformation. Based on calculated values of interface velocities (1.19-4.67 m/s) and mobilities (30-40 kJ/mol), we identify the mechanism of $\gamma - \alpha$ transition studied in this paper as massive transformation. We clearly show that the disconnections act as the nucleation centers for the ferrite phase. Interestingly, higher concentration of such defects at the interface enhances the rate at which austenite transforms to ferrite. Moreover, in the absence of disconnections, atomically flat interface between $\alpha$-Fe and $\gamma$-Fe (formed according to NW ORs) remains immobile and the two solid phases coexist for the entire span (up to 20 ns) of the molecular dynamics simulations. This clearly proves that defects are crucial for the transformation to start and disconnections are certainly a type of defect which can assist in this regard.

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