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# Effect of pre-existing defects in the parent fcc phase on atomistic mechanisms during the martensitic transformation in pure Fe: A molecular dynamics study

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ABSTRACT

Molecular dynamics (MD) simulations are used to study the effect of different defect configurations and their arrangements in the parent fcc phase on atomistic mechanisms during the martensitic transformation mechanisms in pure Fe. The defect configurations considered are stacking faults (SF) and twin boundaries (TB) in single crystal fcc. Three arrangements of these defect structures are considered: parallel TB, intersecting SF, and intersecting SF and TB. Each of these defect configurations affect the transformation mechanisms and transformation temperatures. Parallel TB are the lowest-barrier sites for the atomic shear and thus accelerate the transformation process. The fcc phase with parallel TB follows the Nishiyama-Wasserman (NW) martensitic transformation mechanism. On the other hand, intersecting SF impede the atomic shear and thus retard the transformation. The atomistic transformation mechanism in this case first follows the hcp to bcc Burgers path and then the fcc to bcc Olson-Cohen model. The intersecting SF and TB result in a combined effect of both the previous cases. The simulation results show the occurrence of different atomistic mechanisms during martensitic transformation depending on the type of defects present in the parent fcc phase.



## 1. Introduction

The martensitic transformation mechanisms represent a diffusionless type of phase transformation in many material systems such as Zirconia, Titanium, and some Cu alloys. The martensitic transformation involves a coordinated and ordered rearrangement of the atomic configuration [1]. In Fe-C alloys the martensitic transformation represents the change in crystal structure from face-centered-cubic (fcc) austenite to body-centered-cubic (bcc) or body-centered-tetragonal (bct) martensite. This mechanism mainly occurs by the displacive motion of atoms during rapid quenching and plays an important role in the mechanical properties of Fe-C alloys.

The engineering importance of the martensitic transformation has led to significant efforts to explore its transformation mechanisms. Different theoretical models have been proposed in the literature to explain the transformation process, such as Bain model, shear models by Kurdjumov-Sachs (KS) and Nishiyama-Wasserman (NW), a hard sphere model by Bogers-Burgers (BB), and the Olson-Cohen (OC) model which is based on the BB model (BB/OC) [2–7]. Recently a phenomenological theory of martensite transformation (PTMT) and a two step theory by Cayron have been proposed [1,8]. The Bain model considers the lattice expansion in two fcc lattice directions and contraction in the third to achieve the bcc crystal symmetry. The NW and KS models consider atomic shear on alternate {111} planes with $[11\bar{2}]$ and $[10\bar{1}]$ fcc directions being invariant, respectively. The BB/OC theory describes the crystal structure change as the nucleation of the bcc phase at the intersection of two stacking faults on two {111} planes. The PTMT considers the transformation as a matrix multiplication in two steps: a first step, called invariant plane strain, responsible for the macroscopic shape change and a second step involving shear, to change the crystal structure without shape change. According to PTMT theory the resultant martensite has a twinned structure. The PTMT theory rationalizes the martensitic transformation based on the generation of twinned martensite to accommodate the shape and crystal structure change. The two-step theory considers the atomic displacements by introducing a new parameter called the angle of planar distortion. The details of these models can be found

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in the literature [1,6,7].

The above theories are all based on lattice transformation models and do not take into account the exact atomic displacements during the transformation process, except for the BB/OC model. The BB/OC model considers both the atomic displacements and the transformation process as resulting from the passage of two partial dislocations [8,9]. They also do not consider the effect of pre-existing defects in the parent fcc phase on the martensitic transformation. The different defect structures such as dislocations, stacking faults (SF) and twin boundaries (TB) are important as they are present in the high temperature fcc phase of Fe based alloys depending on the exact alloy composition and the applied heat treatment [1,7,10–12]. Furthermore, in experimental studies it is difficult to separate the effect of each type of defects since more than one defect type will be present at any given temperature in the macroscopic polycrystalline samples. Theoretical models have therefore been difficult to validate and analyse thoroughly at the atomic scale in experiments. The difficulty in analysis also arises from the fact that one or more processes (such as slip, twinning, and shear) can occur simultaneously that are difficult to analyse and correlate. In addition, in-situ observations at the atomic scale are not feasible. Few experimental studies have reported the transformation mechanisms but their results are deduced based on the final microstructure observed [7,11,12]. The details of atomic movements during the transformation process cannot be observed experimentally.

In 1971, Krauss et al. studied the morphology of martensite in various Fe alloys [13]. They concluded that the phenomenological and crystallographic theories of martensitic transformation mainly consider the lattice-invariant deformations. These theories do not consider factors such as the role of austenite and the defects present in the austenite during the shear processes, stacking fault energy of austenite, and the ability of austenite to be stable with respect to the newly forming martensite. Recently, considerations have been given to understand the effect of stacking fault energy changes due to alloying additions on the mechanical properties of steels [14,15]. But other questions are still largely unexplored.

Atomistic simulations methods such as molecular dynamics (MD), have evolved as a powerful tool to analyse the mechanisms which are difficult to observe experimentally. MD simulations have been used to study different aspects in Fe based alloys such as the fcc to bcc transformation at fault intersections by Sinclair et al. [16] and in systems containing bcc/fcc interfaces [17–19]. Wang et al. have studied temperature induced martensitic phase transformations in single crystal Fe-C alloys using MD simulations [20]. They studied the effect of different parameters such as heating and cooling rates on the transformations, and benchmarked these parameters to observe the transformations. They have also discussed the effect of C addition on the transformation temperatures and evolution of stress during transformation. However, they have not discussed the martensitic phase transformation mechanisms in terms of atomistic processes.

The present MD study aims to observe the precise atomic displacements associated with the fcc to bcc transformation during thermal quenching in presence of pre-existing defects in the parent fcc phase. We aim to answer some of the above questions, related to the role of austenite and the defects inside it on the martensitic transformations, on the basis of the MD simulations on pure Fe. In particular we focus on the atomic shear that takes place in the parent fcc austenite phase in presence of defects and the role of austenite transforming to martensite. The defect structures considered here are planar defects such as SF and TB in the parent fcc phase.

The paper is organized as follows. In Section 2, we introduce the simulation methodology and defect structures in the parent fcc phase developed during heating. In Section 3, we will discuss the phase transformation mechanisms from fcc to bcc during cooling. Section 4 describes and discusses the effect of defect structures on the transformation mechanisms and transformation temperatures.

## 2. Simulation methodology

The choice of interatomic potential is most critical for MD studies. We have used the Meyer-Entel embedded atom method potential for the simulations in the present work [21]. Engin et al. [22] characterized six different embedded atom method (EAM) type potentials in the literature to conclude that only the Meyer-Entel potential can describe both the bcc-to-fcc and fcc-to-bcc transformation. The Meyer-Entel potential has been used in the literature previously to study the fcc and bcc phases in pure Fe [20,23–25]. The limitations of this EAM type potential is that it does not consider the magnetic effects which play an important role in the thermodynamic and equilibrium properties of Fe. Although this influences the relative stability of the two phases, the transformation mechanisms can be assumed not to be influenced by this shortcoming [26]. This potential predicts that the atomic volume of fcc is greater than bcc, since the lattice constant of fcc phase for this potential is 3.686 Å whereas experimentally it is found to be 3.571 Å [27]. The implication of the slightly higher atomic volume is that a volume increase is observed during bcc-to-fcc transformation and a decrease is observed during fcc-to-bcc transformation, which is opposite to what is observed experimentally. Song et al. studied the nucleation kinetics of the bcc phase at the grain boundaries of fcc nano-polycrystalline Fe with a potential which shows the opposite trend for the fcc-bcc volume change and found that this discrepancy does not affect the nucleation and growth of the bcc phase at the fcc grain boundaries [28]. In addition, we also calculated the stacking fault energy (SFE) of the fcc phase of Meyer-Entel potential along the $\{111\}<112>$ slip system. The SFE value is -54 mJ/m$^2$. Two recent first principles studies on the fcc Fe mention that the SFE value of non-magnetic fcc Fe is -415 mJ/m$^2$, whereas for paramagnetic fcc Fe it is -105 mJ/m$^2$ [29,30]. Therefore, we can conclude that the SFE of the Meyer-Entel potential is in much better agreement with the paramagnetic fcc phase even though the EAM formalism of the potential does not consider the magnetism explicitly. The important thing to note here is that the magnitude of the SFE is negative both from the Meyer-Entel potential and first principles data, which indicates a spontaneous formation of the planar defects in the fcc phase. The SFE of the modified embedded atom method (MEAM) type potential by Lee et al. for the fcc phase was found to be positive (+37.5 mJ/m$^2$) in opposite trend to the first principles data [31,32], therefore we do not use this potential. For the present work, it is very important to have the correct energetics of the planar defects, in this case SF, with respect to the first principles data; because it is this energetics that controls the stability of the planar defects in the fcc phase. The presence of stable planar defects will in turn have an effect on the atomistic transformation pathways. Considering these arguments, literature studies, and the matching of the SFE value with the first principles data, we use the Meyer-Entel potential in the present work to analyse the effect of planar defects on the fcc-to-bcc transformation process.

The supercell used for pure Fe as the starting point of the simulations is a single crystal bcc system with periodic boundaries in all three directions. The supercell sizes used are 15*15*15 and 20*20*20 unit cells in X, Y, and Z directions, respectively. NPT ensemble is used to control the temperature and pressure of the simulation system. First the energy minimization of the supercell is done at 0 K to obtain the correct lattice constants and energy of the system. The system is then equilibrated at 50 K for 100 ps so that