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Simulation of the massive austenite–ferrite transformation under uniaxial loading

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ABSTRACT

The massive austenite–ferrite phase transformation has been simulated on an atomic scale by means of a multi-lattice kinetic Monte Carlo method. The simulated system involved a ferrite–austenite bicrystal under various uniaxial loads and for a variable number of vacancies at the interface. The results show that the massive transformation from austenite to ferrite is controlled by the local rearrangement of austenite atoms initially blocking unoccupied ferrite lattices sites. The growth mode is strongly dependent on the orientation of the interface. The effects of loading and vacancy concentration at the interface are discussed in terms of their impact on the necessary local rearrangement of austenite atoms. It is shown that local, relaxed clusters of atoms surrounding a vacancy play an important role for the kinetics of the transformation.

1. Introduction

The functional and structural engineering properties of a (metallic) workpiece are determined by its microstructure. A very important, much applied way of changing the microstructure of a solid material is to subject it to a solid state phase transformation [1,2]. The massive austenite (γ) → ferrite (α) transformation is one such transformation for iron-based alloys. The massive transformation is characterized as an interface-controlled transformation, where the austenite–ferrite hetero-interface migrates through uncorrelated jumps of atoms across the phase boundary; i.e. in the absence of long range diffusion. No special Orientation Relationship (OR) between parent and product phase occurs [3–5].

In situ experimental studies of the kinetics of the massive austenite–ferrite transformation are usually of macroscopic nature (i.e. length/volume or enthalpy changes are recorded) [6–11]; microscopic, atomistic data are commonly obtained only after the transformation has been completed, also because of the usually high transformation rates at the elevated temperatures; e.g. the austenite transformation is completed within a few seconds at temperatures in the range of 1090–1120 K [10]. The effect of uniaxial loading on the massive austenite–ferrite transformation has been investigated for FeNi alloys [9,11]. It was shown that uniaxial compressive loading decreases the transformation induced deformation energy, so that the interface velocity increases with increasing compressive stress. For increasing uniaxial tensile loading it was shown that the transformation induced deformation energy increases, so that the interface velocity decreases with increasing tensile stress. These effects were ascribed to anisotropy of the distribution of strain. As a uniaxial compressive load causes compression in the same direction as the load axis and expansion in the two normal directions, the transformation is facilitated in the directions normal to the load axis more than that the transformation is suppressed in the direction parallel to the load axis. For tensile loading the case is reversed: the transformation is suppressed in the two directions normal to load axis more than that transformation is facilitated parallel to the load axis [11].

The mechanisms controlling the massive transformation are inherently of atomistic nature. In view of the experimental difficulty to reveal the atomistic mechanisms in a direct way (see above) atomistic simulations can provide fundamental insight on the atomic time and length scales. Atomistic simulation of the austenite–ferrite phase transformation has been performed by either Molecular Dynamics (MD) methods [12–15] or kinetic Monte Carlo (kMC) methods [16–19]. Using a MD approach to investigate the massive transformation would need a driving force (which is given by/derived from the employed atomic interaction potential) for the transformation that low that the martensitic transformation does not occur [3], while the driving force should be high enough for the (desired) massive transformation to be completed in MD time scales [16]. These constraints can practically, for general interfaces, not be met. Therefore employing a

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kMC method, with an inherently non-coordinated movement of atoms and an accessibility to much longer time scales, appears to be very appropriate for simulation of the massive austenite–ferrite transformation.

KMC simulations by Bos et al. [16–19] show that the activation energy of the interface mobility is governed by the amount of (excess) free volume and its distribution at the hetero-interface. The (excess) free volume is necessary to enable the movement of atoms away from austenite–lattice sites blocking ferrite–lattice sites. The free volume was varied in these studies by the insertion of vacancies at the interface region.

(Metallic) workpieces/components in practice are subjected to applied or residual stresses, which can have great influence on (the kinetics of) phase transformations [10,11]. The effects of stress on the massive austenite–ferrite transformation have not been investigated until now by atomistic simulations. The goal of this work is to investigate by kMC simulations the role of uniaxial tension and compression and excess free volume (by introducing vacancies) on the interface mobility of the austenite/ferrite interface.

2. Simulation of transformation kinetics

The (kinetic) Monte Carlo method involves the creation of a catalogue of possible events from which an event is chosen stochastically to happen and the consequences of the chosen event are evaluated. This approach has been adopted here to investigate the (interface) kinetics of the massive $\gamma \rightarrow \alpha$ phase transformation. The individual events considered in the simulation are the jumps of atoms from their initially position to an empty site in discretised space. In contrast with the common kMC simulations, where only one crystal lattice is used, a multilattice kMC method [16,17] is used in this work: the possible positions of the atoms are provided by the sites of the crystal lattices of the parent phase and the product phase plus a certain amount of so-called random sites that the atoms can take for an intermediate position between the crystal-lattice sites. Providing these intermediate positions is essential for a realistic description of the transformation interface: at and close to the interface neither the atoms take positions precisely as prescribed by the lattices of the adjacent crystals nor do they go over from an austenite–lattice site to a ferrite–lattice site by one atomic jump. These random sites are distributed adopting a restrictedly random distribution method, by dividing the simulation volume in cubic cells with an approximate edge length of the second nearest neighbour distance in the γ phase and randomly distributing a fixed amount of random sites per cell.

The simulation loop starts with creating a list of all interface atoms. An atom is defined as an interface atom if it is adjacent to an atom of another type or if there is a vacancy on one of the neighbouring sites of its own type. For all these interface atoms all the possible jumps and corresponding jump rates are calculated. The jump rate k_i for jump i is calculated by

$$k_i = \nu_0 \exp\left[-\frac{E_i^a}{k_b T}\right] \tag{1}$$

where ν_0 is a frequency factor, E_i^a is the activation energy for jump i, k_b is the Boltzmann constant and T is the (absolute) temperature. The activation energy E_i^a is determined by $Q_i + \Delta U_i$, if the energy difference between the new configuration and the original configuration, ΔU_i, is positive, and by Q_i otherwise. Here Q_i represents the energy barrier for jump i, which is dependent on the local surroundings of the jumping atom.

The energy difference ΔU_i between two configurations is calculated via the Embedded Atom Method (EAM) [20,21] using the Johnson-Oh potential [22].

The energy barrier Q_i is calculated with the Locally Activated Monte Carlo (LAMC) method [23]. This is a procedure in which the jumping atom is moved in small steps along a straight line from its starting position to its destination. After each step, the jumping atom and the (here) 14 closest atoms to the straight line between start and final position of the jumping atom are allowed to relax according to the conjugate gradient method [24]. During the relaxation the jumping atom is allowed to move only in the plane perpendicular to the straight line mentioned before. After the relaxation the cohesive energy of the system is stored. The difference of the cohesive energy associated with the state with the highest (=least negative) cohesive energy, along the path mentioned, and the cohesive energy associated with the start configuration is the activation energy E_i^a. If the cohesive energy difference ΔU_i is negative, the energy barrier Q_i is equal to activation energy, otherwise ΔU_i was subtracted from E_i^a to obtain Q_i. As determining values of Q_i during the Monte Carlo procedure would increase the simulation times dramatically, a neural network was trained to give a value for Q_i (output parameter) with a given set of input parameters. A suitable set of input parameters consists of the jump distance, the cohesive energies before and after the jump and the positions of the fourteen nearest neighbours.

A data set, containing the input parameters and the output parameter for 35,000 jumps in the stress-free system, was used to train the neural network. Using a separate data set, containing the input parameters and the output parameter of another 5000 jumps in the stress-free system, to validate the trained neural network, yielded a normalised root mean square error for Q_i of less than two percent. For each of the states of stress applied in this work a data set, consisting of the input parameters and their corresponding output parameter as calculated for a certain number of jumps by the LAMC method, was created. These data sets for strained bicrystals were used to validate the neural network, trained for the stress-free system, for application to strained bicrystals. It followed that the maximum normalised root mean square error in the value of Q_i is less than 8%.

After the determination of the jump rates for all possible jumps for all interface atoms, these jump rates are summed up to a total jump rate K_{sum}

$$K_{sum} = \sum_i^N k_i \tag{2}$$

where N is the total number of jumps of all interface atoms. Next a random number R_1 between zero and K_{sum} is chosen. The jump selected to happen then is the first jump a for which the sum of its jump rate k_a and the jump rates for jumps with lower indices is equal to or larger than R_1:

$$\sum_i^a k_i \geqslant R_1 \tag{3}$$

The time Δt between two successive jumps can be calculated [25] using K_{sum} and a second random number R_2 between zero and one:

$$\Delta t = \frac{\ln(R_2)}{K_{sum}} \tag{4}$$

Here the basic simulation loop ends. The basic simulation loop is repeated until 50,000 atomic jumps have been made. Next (i) unused random sites are redistributed, again according to the restrictedly random distribution described above and (ii) the γ crystal is moved to accommodate the volume misfit between both phases. The misfit is accommodated by moving the γ lattice along the direction normal to the interface (the z-axis in Fig. 1), until the