VOID HARDENING IN BCC-IRON STUDIED BY ATOMIC-SCALE MODELLING—

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OBJECTIVE

The objective of this work is atomic-scale modelling of interactions between moving dislocations and particular obstacles. Two different atomic-scale techniques based on (a) a periodic array of dislocations (PAD) and (2) Green's function boundary conditions (GF) in alpha-Fe are used. to elucidate influence the dislocation-image interaction taking place in the case of PAD. Since the PAD and GFBR methods are quite different, they have been applied to the same problem for comparative study. First results of such a study are presented for motion of dislocation in perfect crystal and in crystal containing a row of 2nm spherical voids in bcc Fe.

SUMMARY

Atomic-scale modelling permits detailed simulation of the interactions between moving dislocations and particular obstacles. Such simulations should be of large enough scale to simulate a realistic dislocation density and obstacle spacing, and correctly treat long-range self-interaction between dislocation segments. Results obtained with a 2 nm void and two different atomic-scale techniques based on (1) a periodic array of dislocations (PAD) and (2) Green's function boundary conditions (GF) in alpha-Fe are presented. Static, zero temperature, simulations have been carried out with incrementally increasing strain until dislocation overcomes the obstacle. It is concluded that both techniques reproduce the same critical resolved shear stress (CRSS), and similar void and dislocation modifications are observed.

PROGRESS AND STATUS

Introduction

The crucial role of dislocations in mechanical properties of materials has been successfully shown by continuum elasticity theory. However, understanding the processes that are controlled by atomic scale mechanisms require development of new modelling techniques. The interaction between gliding dislocations and an obstacle in its glide plane is an example of such a process. One of the most successful models [1] is based on a periodic array of dislocations (PAD) using an approach originally proposed by Baskes and Daw. PAD simulates a crystal containing initially straight edge dislocations with periodic boundary conditions along the dislocation line and in the direction of the Burgers vector. The model allows the correct configuration of the dislocation core structure to be simulated and has been successfully applied to study different type of obstacles in bcc and fcc metals (see e.g. [2, 3]). The model is simple and fast, but some limitations a rise when compared with results from macro-models based on the "single dislocation in infinite media" approach. These appear because of dislocation-image interaction due to periodic boundary conditions along Burgers vector.

Another model proposed recently [4] employs 3D Green's function boundary relaxation conditions (GFBR) [5]. In this method, flexible GFBC are used along the Burgers vector and perpendicular to the slip plane. Periodicity is maintained along the dislocation line only to enable simulating the mobility of a single dislocation and its interaction with an array of obstacles [4, 6]. The simulation cell consists of three regions: atomistic, Green's function and continuum. In the atomic region atoms are displaced according to Newton's equation of motion. As the atomic region is relaxed, forces build up on atoms in the Green's function region, which cause displacements in all three regions (an efficient method to calculate the elastic displacement field was developed in [7]). Atoms in the first region are relaxed in response to the forces followed again by relaxation of whole crystal via GFBC is reached a stable configuration. This model has been used to calculate the interaction of edge dislocation with voids in bcc tungsten [4]. Since the PAD and GFBR methods are quite different, they have been applied to the same problem for comparative study. First results of such a study are presented for motion of dislocation in perfect crystal and in crystal containing a row of 2nm spherical voids in bcc Fe.

Calculation Details

An edge dislocation with Burgers vector ½[111] and {110} slip plane in bcc-iron was simulated using the many-body interatomic potential of Finnis-Sinclair type parameterized in [8]. The calculations by PAD are carried out in crystals containing (2-8)x10^6 mobile atoms whereas GFBC were applied in crystals having ~(0.2-1.0)x10^6mobile atoms. The crystal size is varied in the direction of Burgers vector only to test influence the dislocation-image interaction. To simulate motion of the dislocation a shear strain was incrementally increased with a step equal to 10^{-4}. Each increment was followed by relaxation to the minimum potential energy. For the FBC, each strain increment also was followed by up to 8 relaxation steps of the GF boundary layer. Strain was increased until the dislocation moved over a desired distance or overcame the obstacle. In both types of calculation, a stress-strain curve, critical resolved shear stress (CRSS) and dislocation line shape at the CRSS has been obtained and analysed. The both techniques have been applied at T=0K.

Results

An example of the stress-strain curves calculated for the case of dislocation glide in perfect crystal, together with the dislocation core displacement, is presented in Fig. 1. As can be seen, the stress-strain curves are the same in linear elastic regime, i.e., before the dislocation moves. When the stress reaches a critical value, i.e., the Peierls stress, the dislocation moves and this motion is different in different models. Thus, in the case of PAD model the dislocation motion depends on dislocation density and obeys the Orowan relationship $\varepsilon = \bar{x} b \rho$. In the case of GFBC, when a single dislocation is simulated in the infinite medium, the dislocation moves continuously until interaction with boundaries compensates applied shear stress. Note that in the case of PAD the Peierls stress is the maximum stress generated in the system (curve 2 in Fig. 1) whereas in the case of GFBC the maximum stress can be infinitely high reflecting the repulsive force between the dislocation and a boundary (curve 1 in Fig. 1a). However, the value of Peierls stress calculated in the both cases is the same (τ_P~24MPa) as well as the critical strain: ε_P=0.033% (GFBC) and 0.035% (PAD).

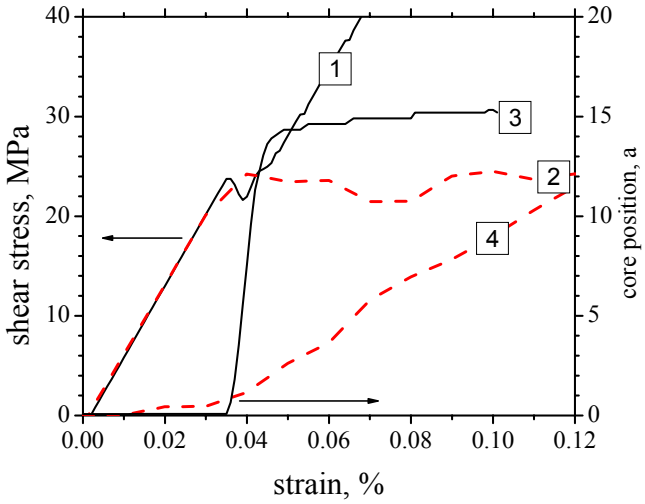

Fig. 1. The stress-strain curves and core positions for the edge dislocation calculated via PAD and GFBC. 1, 2 – stress-strain for GFBC and PAD; 3, 4– core positions for GFBC and PAD.

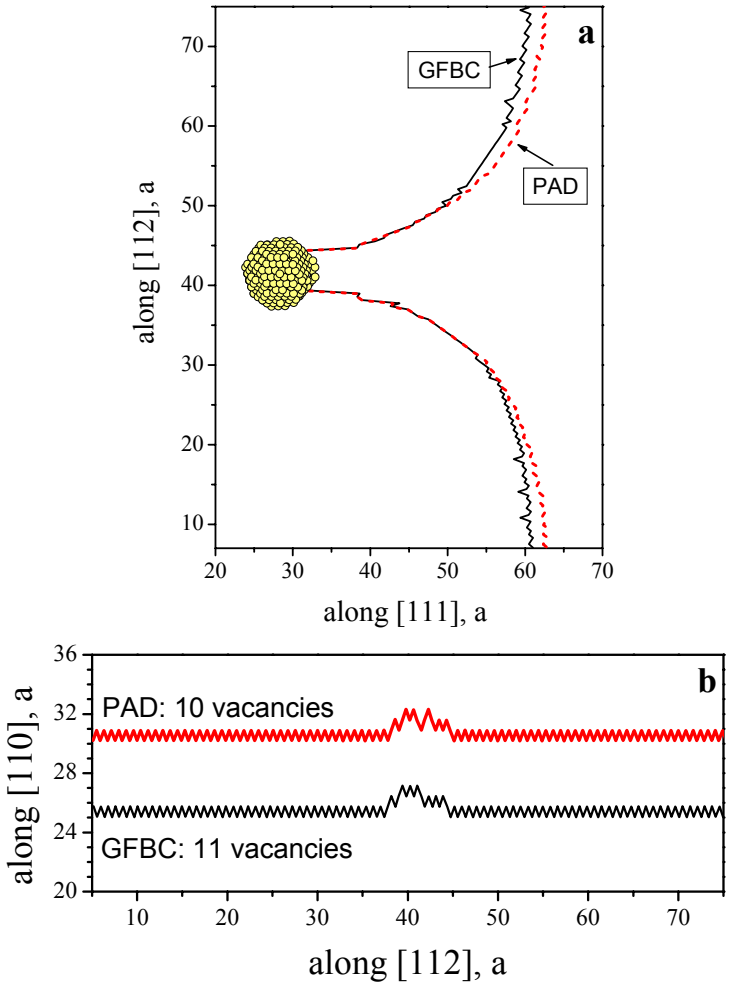

Fig. 2. Comparison of PAD and GFBC calculations for 2nm void at 0K: (a) -dislocation line shape at (b) -critical stress and dislocation climb due to interaction.

In the case of dislocation-void interaction, a full stress-strain curve can be obtained only for the PAD [1, 2]. Therefore, a comparison between the models was made only for the dislocation line shape at the critical condition, i.e., just before it overcomes the obstacle out, and the line shape after the interaction. The former is presented in Fig. 2a where one can see that both lines have very similar shape suggesting that the force distribution related to dislocation-void interaction is also very similar. It was observed earlier that the dislocation absorbs vacancies during the interaction with a void. It is found that in both cases the dislocation absorbs a similar number of vacancies, i.e., 11 for the GFBC and 10 for the PAD, and the shape of superjog created due to climb is also very similar (see Fig. 2b).

Conclusions

Two atomistic-scale techniques, PAD and GFBC, have been used to study dislocation dynamics in perfect crystal and dislocation-void interaction in bcc-Fe. It was found that both techniques lead to similar results: including, the Peierls stress and strain, the dislocation line shape near the void at critical stress and atomic-scale structure of the dislocation line, and void shrinkage after dislocation-void interaction.

References

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