DISLOCATION EMISSION FROM THE CRACK TIP IN BCC IRON

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ABSTRACT

Atomistic simulations under plane strain conditions by molecular dynamic technique (MD) show that microcracks with orientation (-110)[110] can emitt complete edge dislocations in the slip systems <111>{112}. It causes crack tip blunting and stability of microcracks under quasistatic loading in mode I. Motion of the dislocations away from the crack tip is subsonic. The results have been obtained with an N-body potential for α-Fe. Calculations of the stress on atomic level and work done by the stresses are planed to compare the MD results with continuum predictions.

KEYWORDS

Molecular dynamic, α-iron, brittle-ductile behavior at the crack tip

INTRODUCTION

The aim of the work was to study brittle versus ductile behavior near the crack tip. Molecular dynamic technique has been used to examine behavior of microcracks in bcc iron. We consider an atomistic sharp central crack with orientation (-110)[110], embedded in a relatively large sample. Crack is loaded in mode I. Due to symmetry of the problem, only one half of the sample is treated in the simulations. In agreement with anisotropic LFM, we consider plane strain conditions. Different crack lengths, different loading rates and applied stress level has been tested. It is known from experiments that a crack tip can be blunted by a slip of pre-existing dislocations or from emission of new dislocations from the crack tip, which can influence crack stability. The stability (or unstability) of the crack is the key problem for the safety of the construction, and so significant attention is dedicated to the problem using both the continuum model and also the atomistic simulations. These two procedures verify and complement each other. Previous studies with a different crack orientation (001)[110] in [1] have been shown that twin generation is favored at the crack tip under a sufficiently large quasistatic stress [1], or under fast loading [2]. We use the same N-body potential as in [1,2]. In agreement with [3], we confirmed the assumption that for our crack orientation (-110)[110], emission of dislocations occurs more easily than twinning, which causes crack stability.

MD SIMULATIONS

The crystal is oriented in x_1 = [001], x_2 = [-110] and x_3 = [110] directions. Plane-strain in x_3 direction is considered, i.e. $\varepsilon_{33} = \varepsilon_{31} = \varepsilon_{32} = 0$. In this direction the periodical boundary conditions are used and the movement of atoms in x_3 is prohibited. The atoms can move in the directions x_1 and x_2, i.e. the thickness and the width of the sample are not fixed. A symmetrical rectangular sample with a central crack in the central is considered. To simplify the simulation only on half of this sample is treated. To secure the symmetry, the movement of atoms lying at the symmetry axis is forbidden in the cross direction. To select sample dimensions, a similarity with fracture mechanics from continuum has been utilized. For our sample dimensions 600 x 300 atoms and the basic crack length $2.l_0=2.30.a_0/2$, the boundary correction factor F_I for loading mode I corresponds nearly to 1, i.e. the sample is relatively large.

Unlike pair potentials, the used N-body potential describes well the all elastic constants and also energetic. The energy 2γ needed to create a new free surface with the more complicated N-body potentials is calculated as a difference of new descent configuration with free surface and the system in the perfect state. In the case of GA potential [2] the individual values are γ_{001} = 1,812 J.m^{-2}, γ_{110} = 1,585 J.m^{-2} and γ_{111} = 2,269 J.m^{-2}. The critical Griffith stress intensity factor $K_I = K_G$ according to anisotropic LFM is given by the relation $2.\gamma_S = C.K_G^2$, where C is an anisotropic constant for plane strain. The individual values for crack orientations (001)[110] and (-110)[110] are given in Table 1. The orientation denotes crack plane versus crack front. The corresponding Griffith stress is given by the relation $K_G = \sigma_G \sqrt{\pi.l_0}$.

Table 1. Material constants in used directions

Crack orientation	γ_S (J / m^2)	C (10^{-12} m^2 / N)	K_G (MPa . m$^{1/2}$)
(001) [110]	1.812	4.83	0.8662
(-110) [110]	1.585	5.043	0.7928

In molecular dynamic method the Newton's system of equations for particular atoms are solved. For time integration of Newtonian equations, the explicit method with central differences is used. In this method the time step should respect the numerical stability of the system. This condition is fulfilled as far as the time step is smaller than the moment needed to pass the shortest distance in the lattice. The time step 0.01 ps is selected. The thermal motion of atoms is not regulated, i.e. atomic velocities are not prescribed.

Before loading, the sample is relaxed to avoid influence of surface relaxation on microscopic processes at the crack tip. After that, the sample was gradually loaded up to a maximum level σ_A, corresponding either to σ_G or to $1.2\,\sigma_G$ and then the applied stress was held constant. According to premeditation ensue from energetic balance the loading rate can be divide by period of free vibrations T_{110}:

a) Quasi-static – period of loading after 6000 steps > $T_{110}/2$

b) Faster load – period of loading after 1000 steps ≈ $T_{110}/2$

c) Dynamic load – period of loading after 100 steps < $T_{110}/2$

RESULTS AND DISCUSSION

A microcrack with half-crack length $l_0 = 30\ a_0\ /2$ has been preferably studied. In this case, emissions of complete edge dislocations from the crack tip in the slip systems <111>{112} have been observed near by the Griffith stress. The simulation result for quasistatic loading is shown in Fig. 1. Dislocation emission prevented crack extension at this stress level. Under a load $\sigma_A \geq 1.2\ \sigma_G$ just very small plastic growth of microcrack $l_0 = 30.a_0 / 2$ was observed. Even longer cracks were not begun by brittle way. This is a different behavior in comparison with a crack (001)[110] studied before in [1].

Since the graphic output has been printed at different time steps, we can to observe the kinetics of dislocation motion away from the crack tip and to determine dislocation speed. The maximum calculated speed of dislocations was 2482 $m.s^{-1}$, which is less than the corresponding velocity of shear waves 3007 $m.s^{-1}$ in the slip system <111>{112}. In the next part we will compare our results with the atomistic results by other authors and with continuum predictions on the brittle-ductile behavior.

Atomistic simulations

Equivalent orientation of the model, loading, similar potential but different boundary conditions and a long crack in the work [4] is used. Authors in [4] observed brittle initiation of the crack in α-Fe with value of K_{IC} slightly higher than K_G. Shastry and Farkas in [3] report dislocation emission from a microcrack with our orientation below Griffith stress. It is important, that these results have been obtained with different potential and different boundary conditions. For our crack orientation, it is possible to state: microcracks with a large σ_G can emitt dislocations, while long cracks with small σ_G can be initiated via cleavage by Kohlhoff et al. [4].

The same N-body potential and boundary conditions have been used in [1] to study brittle-ductile behavior at the crack tip of a (001)[110] microcrack. Atomistic results and as well global energy and force balance in [1] have been shown that in this case twinning in the slip systems <111>{112} is more favorable than dislocation emission from the crack tip. The different behavior of the cracks (001) and (-110) is possible to explain qualitatively by a fact that due to orientation the dislocation emission in the slip systems <111>{112} from the (-110) microcrack occurs in the anti-twinning direction, which is not favorable for twinning.

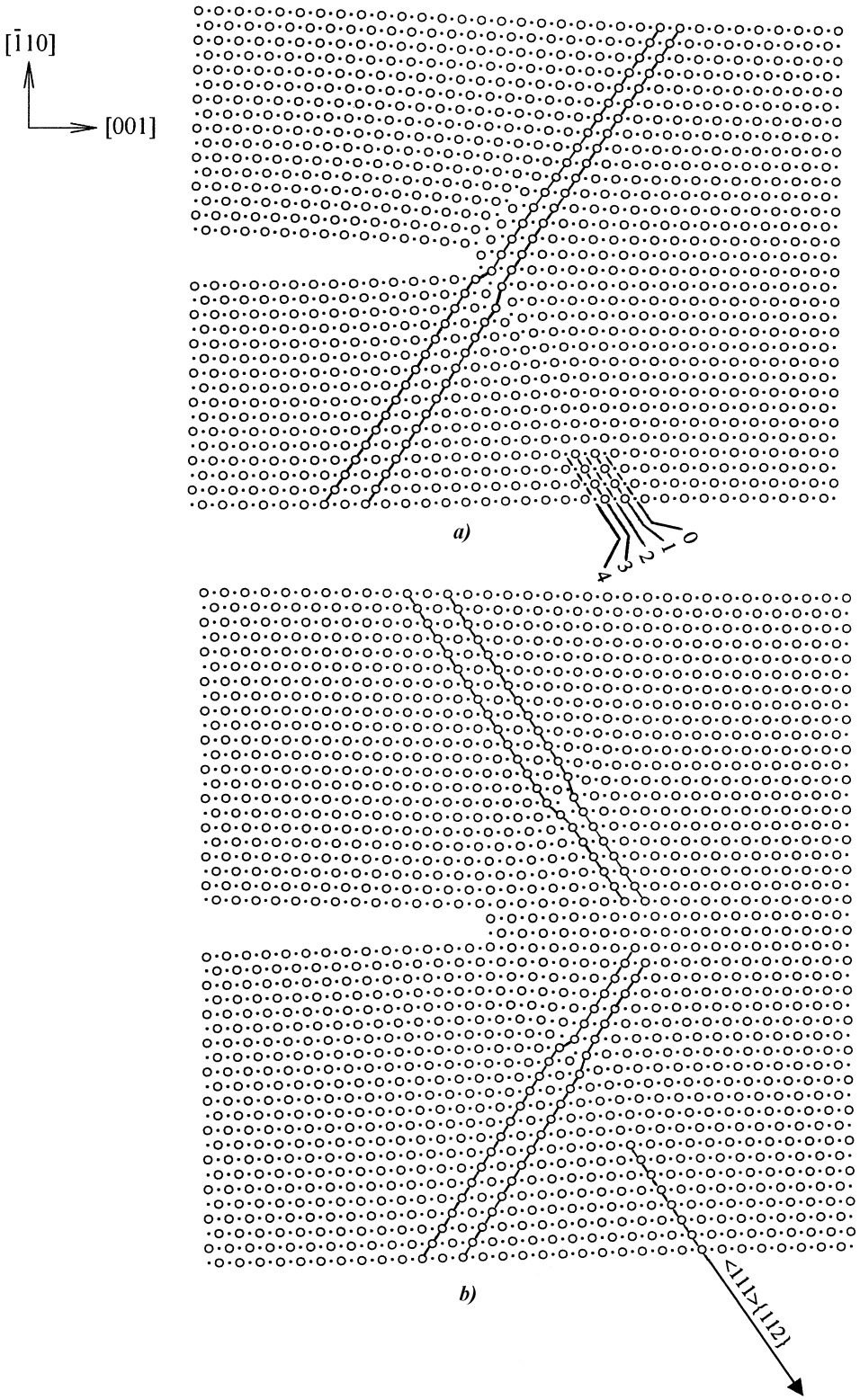

Fig. 1. Detail of atomic configuration near the crack tip during quasistatic loading in time step a) 6500 and b) 6549, $\sigma_A = \sigma_G$

Comparison with continuum models

According to Rice´s model [5] for dislocation emission it is necessary to overcome the energy barrier given by the unstable stacking fault energy γ_{US}. The value γ_{US} = 1.14 J.m^{-2} for the slip system <111>{112} has been determined for our GA potential in [1]. It corresponds to the maximum in global energy balance during block like shear of a perfect bcc iron crystal along the <111>{112} slip system. The critical shear (peak) stress during the rigid sliding corresponds to ideal shear strength τ_p = 16,35 GPa. According to Rice model [5], dislocation emission is favored if $G_{disl} = g(\theta).\gamma_{US}$ is smaller than $2.\gamma_S$. The angle function for our crack orientation (-110)[110] corresponds to $g(\theta)$ = 7,607 and G_{disl} = 8,67 J.m^{-1}, while surface formation energy is $2.\gamma_{110}$ = 3.17 J.m^{-1} (see Tab. 1.). It is clear that we obtain a discrepancy between atomistic results and Rice continuum prediction, similar to [3]. Comparison with an older KTC criteria and new prediction by Beltz, Lipkin and Fisher [6] is still not fully possible, since we do not know the ideal tension strength in the [-110] direction and as well the atomic stresses at the crack tip during simulations. The work will continue in this field.

SUMMARY

Atomistic simulations under plane strain conditions by molecular dynamic technique show a strong dependence of the brittle-ductile behavior on crack orientation. While (001) [110] cracks can be initiated in a brittle way [1] (or with concomitant twinning at the crack tip), the cracks with orientation (-110) [110] emitted dislocations, which caused crack blunting and crack stability near the critical Griffith stress. Movements of dislocations appearing at the crack tip with our crack orientation are subsonic. According to the molecular dynamics, only slow and plastic growth of the crack (-110)[110] at stresses significantly larger than the critical stress is possible. These atomistic results are in agreement with experimental observations that brittle fracture in bcc iron and ferritic steels is observed on (001) planes [7].

ACKNOWLEDGEMENTS

The diploma work from CTU Prague was supported also by the grant A2076701 at AS CR.

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