Sample geometry and the brittle-ductile behavior of edge cracks in 3D atomistic simulations by molecular dynamics

PELIKÁN Vladimír[a], HORA Petr[b], MACHOVÁ Anna[c], KOLMAN Radek[d] and UHNÁKOVÁ Alena[e]

Institute of Thermomechanics AS CR v.v.i., Prague, Czech Republic

[a]pelikan@cdm.cas.cz, [b]hora@cdm.cas.cz, [c]machova@it.cas.cz, [d]kolman@it.cas.cz, [e]uhnakova@it.cas.cz

Keywords: bcc iron, crack growth, dislocation emission, twins

Abstract. We present new results of molecular dynamic (MD) simulations in 3D bcc iron crystals with edge cracks (001)[010] and (-110)[110] loaded in *mode I*. Different sample geometries of SEN type were tested with negative and positive values of T-stress according to continuum prediction by Fett.

Introduction

Crack (001)[010] (crack plane/crack front) under monotonic uniaxial tension can produce dislocations in 3D bcc iron crystals [1] in the available inclined slip systems <111>{101}, while the crack (-110)[110] can emit dislocations in the inclined slip systems <111>{112}, both under monotonic tension [2-3] or cyclic loading [4] in mode I. It occurs at low temperature [2] but also at room temperature [3,4] as experiments on iron crystals [4-5] confirmed. However, ductile behavior at the crack front depends not only on the stress intensity K_I but also on so-called T-stress acting parallel to crack plane [2,7]. Our *previous* molecular dynamic (MD) simulations [2,6,8,9,10] with *central cracks* have been shown that the sign of T-stress influences their brittle-ductile behavior under loading in mode I. Negative T-stress supports dislocation emission [2] or twin generation [10] at the crack tip, while positive T-stress may lead to cleavage fracture [2,9]. It can be easy understood by Rice prediction for inclined slip systems: $\tau_{crit} = \tau^0_{crit} + T \sin(\alpha) \cos(\alpha)$, where τ_{crit} is the stress barrier for the slip process and α is the inclination angle of the slip system with respect to the axis of potential crack extension. Here we present *new MD results* focused to 3D bcc iron crystals with short *edge cracks* (negative T-value) and longer cracks with positive T-stress according to static predictions for isotropic continuum by Fett [7].

MD simulations

We consider a pre-existing edge crack of the length *a* placed in the middle of a rectangular sample of the length *L*, width *W* and thickness *B*. Edge cracks with orientation (-110)[110] and (001)[010] are studied in atomistic samples with the geometries *a/W*, *L/W* and *B/W* accessible for fracture experiments. The samples are loaded by monotonic uni-axial tension (mode I) via external forces distributed in several surface layers in *L* direction. Surface relaxation has been performed before loading to avoid its influence on crack tip processes. The same N-body potentials for bcc iron from [11] have been used in this study as in our previous work. Newtonian equations of motion for individual atoms were solved by a central difference method using time integration step h=1E-14 s.

Edge crack (001)[010] was created by removing 1 layer of atoms in the direction *W* of potential crack extension. Number of atomic layers (001) in *L*-direction is 4999, in *W*-direction it is 1001, and along the crack front (in *B*-direction) it is 201. Total number of atoms in the perfect 3D cubic crystal corresponds to NPOIN = 252 702 000 and parallel processing in MPI was used in this case. At initial temperature of 0 K, systematic studies with different ratios a/W = 0.1,…,0.9 have been performed with loading rate where critical Griffith stress intensity K_G was reached during 15000 h. At temperature of 300 K, the ratios a/W = 0.2,…,0.8 were treated. Beside free 3D simulations, periodic boundary conditions along crack front were also tested with the crack (001)[010].

Edge crack (-110)[110] was created by cutting interatomic bonds across the initial crack plane as in [2,3]. Two different geometries with $a/W = 0.3$ and $a/W = 0.8$ have been studied with negative and positive T-stress by Fett [7]. Initial temperature was 0 K and further thermal atomic motion was not controlled. Atomistic sample consists of 440 atomic planes (-110) in L-direction, 220 planes (001) in W-direction and 30 planes (110) in B-direction along the crack front. Total number of atoms in the 3D crystal is NPOIN = 1 452 000 and sequence processing was used to integrate Newtonian equations of motion with the same time step h = 1E-14 s as above. Loading rate corresponded to K_G per 4000 h.

Results and discussions

Stress field in front of an atomically sharp crack in linear (elastic) phase of loading can be described satisfactory well [2] by linear elastic fracture mechanics (LEFM). In anisotropic continuum at distance r from the crack tip along the axis of crack propagation (angle $\theta = 0$) we may write

$$\sigma_{xx} = -\frac{\mathrm{Re}(\mu_1\mu_2)K_I}{\sqrt{2\pi r}} + T \quad , \qquad \sigma_{yy} = \frac{K_I}{\sqrt{2\pi r}} \quad , \tag{1}$$

where $\mathrm{Re}(\mu_1\mu_2)$ is an anisotropic factor depending on crack orientation. Under plane strain conditions prevailing in the middle of the crystal, - $\mathrm{Re}(\mu_1\mu_2) = +0.8857$ [2] for crack orientation (-110)[110], while for (001)[010] it is - $\mathrm{Re}(\mu_1\mu_2) = +0.99995$, i.e. close [1] to isotropic case with - $\mathrm{Re}(\mu_1\mu_2) = +1$.

Free 3D simulations with edge cracks (001)[010] at 0 K and 300 K have been shown that the brittle-ductile behavior along the crack front is not influenced significantly by the initial crack length, i.e. by T-stress, which is illustrated by Fig.1 and Fig.2. Fig. 1 shows plastic crack growth at temperature of 0 K for crack length $a/W = 0.3$ with negative T according the parameter $(1\text{-}a/W)^2$ $T/\sigma_A = -0.299$ by Fett [7]. Fig.2 illustrates plastic crack growth in the middle of the crystal at 300 K for $a/W = 0.8$ with positive T given by the Fett parameter = +0.233 [7] for the constant applied stress σ_A at the borders and the ratio $H/W = 1.5$ where $H = L/2$. The arrow denotes the original crack tip atoms. In all the cases, crack initiation is accompanied by emission of dislocations in inclined slip systems <111>{101}, visible in Fig. 2 under angle of about 45° by means of the slip patterns with two black atoms [1].

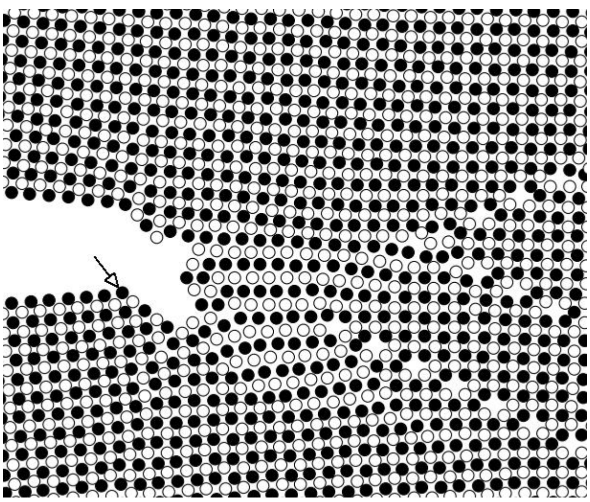

Fig. 1

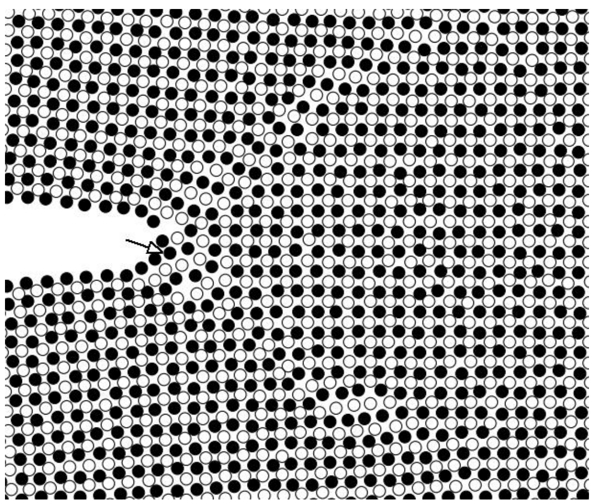

Fig. 2

In 3D, dislocation emission starts from the corners (Fig.3) where the crack front intersects the free sample surface (yellow atoms) since here the stress concentration is higher than in the middle of the crystal [1]. Curved dislocations (red atoms) of mixed character with edge and screw components are emitted [6]. Screw segments may change the slip plane from (101) to oblique (112) plane (see Fig.7 in [1]) which is visible in Fig. 1 by means of empty (vacancy) patterns <111>{112} in front of the crack. *Periodic boundary conditions* along crack front (Fig.4) lead to fast brittle crack extension independently on crack length and temperature.

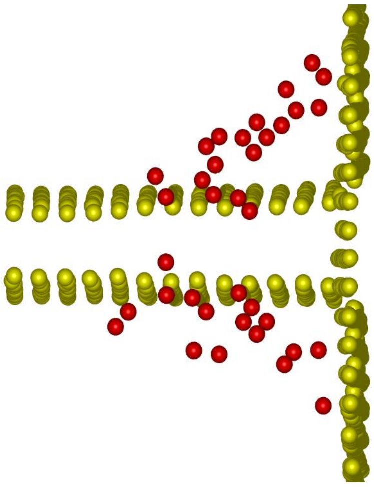

Fig. 3

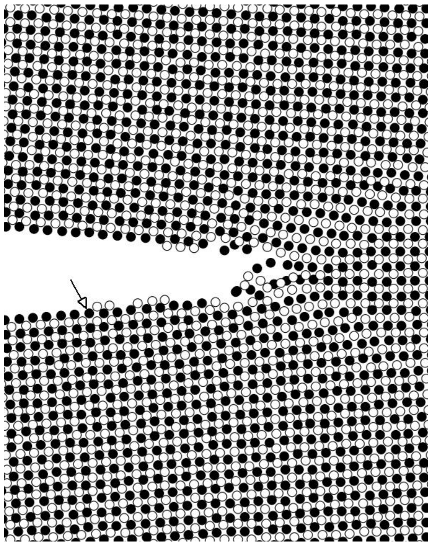

Fig. 4

Edge crack (-110)[110] with ratio $a/W = 0.3$ at temperature of 300 K emits blunting dislocations into the inclined slip systems <111>{112} which leads to a slow plastic crack growth in MD [3] and as well in experiments [5]. *Here* we presents MD results with initial temperature of *0 K* for the crack length corresponded to a/W = 0.3 (negative T) and a/W = 0.8 with positive T by Fett as mentioned above. The short crack $a = 0.3W$ at 0 K emitted dislocations similar to 300 K [3] and the slow plastic crack growth has been realized via the blunting mechanism as in [3,5]. The longer crack $a = 0.8\ W$ emitted also first the blunting dislocations <111>{112}- see Fig. 5.

Later, when the dislocations arrive to the free sample surface creating surface jogs, new stress concentrators cause generation of twins in the easy twinning direction from the free surface toward to the crack front- see Fig. 6. This is the only difference in comparison with the short crack.

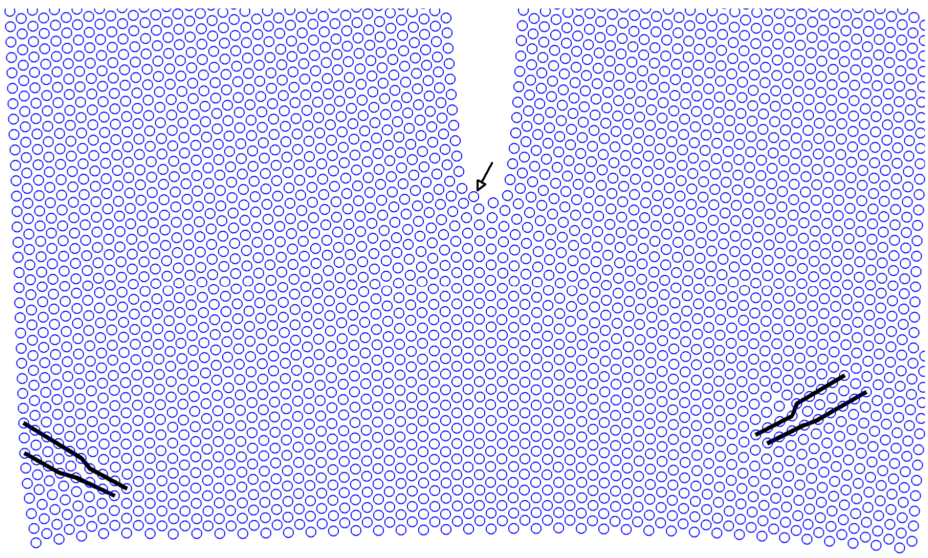

Fig. 5

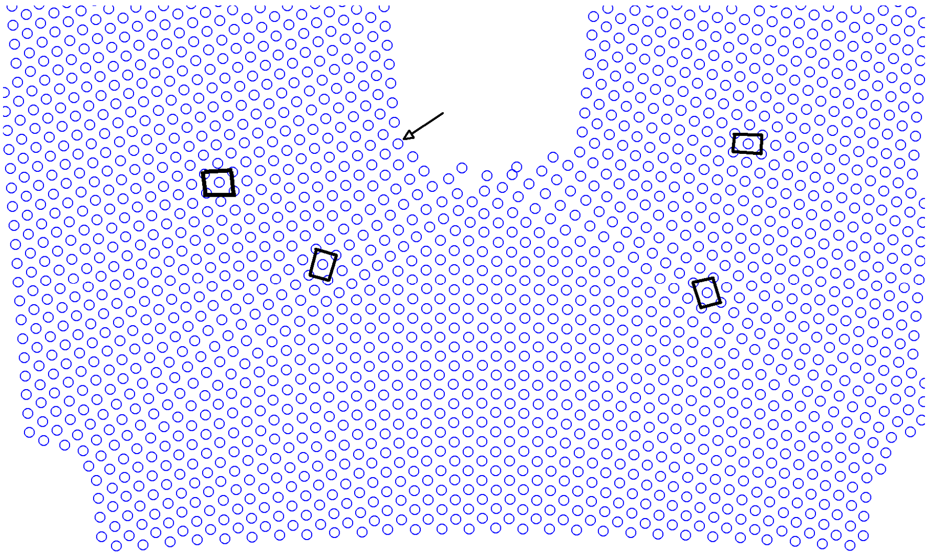

Fig. 6

The both edge cracks demonstrate ductile behavior, although the sign of T-stress differs according to static predictions for isotropic continuum by Fett [7]. Additional stress calculations on the atomistic level have been shown that while the near stress field in front of the short crack *a/W* = 0.3 can be satisfactory well described with negative T and by the LEFM approximation given above, it is not valid for *a/W*= 0.8 where atomistic results indicate negative T instead of positive value by Fett [7]. Possible reasons for the discrepancy are: larger bending under constant stress conditions at the larger crack and more intensive influence of the dynamic effects close to free sample surface.

Acknowledgements: The work was supported by the pilot project IT ASCR No. 904168 with Institutional support RVO: 61388998. The work of A. Machova was also supported by the project of the Czech Science Foundation GACR 15-20666S.

Literature References

[1] V. Pelikán, P. Hora, A. Machová, A. Spielmanová: Czech. J. Phys. B Vol. 55 (2005), p. 1245

[2] G.E. Beltz and A. Machová: Modelling Simul. Mater. Sci. Eng. Vol. 15 (2007), p.65

[3] A. Spielmannová, A. Machová, P. Hora: Materials Science Forum Vol. 567-568 (2007), p. 61

[4] M. Landa, A. Machová, A. Uhnáková, J. Pokluda, P. Lejcek: Int. J. Fatigue Vol. 87 (2016), p. 63

[5] A. Spielmanová, M. Landa, A. Machová, P. Hausild, P. Lejcek: Mater. Charact. Vol. 58 (2007), p. 58

[6] P. Hora, V. Pelikán, A. Machová, A. Spielmannová, J. Prahl, M. Landa, O. Červená: Engineering Fracture Mechanics Vol. 75 (2008), p. 3612, ECF16

[7] T. Fett: *A compendium of T-stress solutions* (Forschungscentrum Karlsruhe GmbH, 1998)

[8] A. Uhnáková, A. Machová and P. Hora: Key Engineering Materials Vol. 465 (2011), p. 69

[9] A.Uhnáková, A. Machová, P. Hora, J. Cerv, T. Kroupa: Comput. Mater. Sci. Vol. 50 (2010), p. 678

[10] A. Machová and G. E. Beltz: Mater. Sci. Eng. A Vol. 387-389 (2004), p. 414

[11] G.J. Ackland, D.J. Bacon, A.F. Calder and T. Harry: Phil. Mag. A Vol. 75 (1997), p. 713