COMPUTATIONAL MECHANICS 2009
25th conference with international participation
Hrad Nečtiny
November 9 - 11, 2009

Ductile–brittle behavior at cavities in 3D iron crystals and in Fe-Cu system

V. Pelikán[a,*], P. Hora[a], O. Červená[a], A. Spielmannová[b], A. Machová[b]

[a] *Institute of Thermomechanics of the ASCR, v.v.i., Veleslavínova 11, 301 14 Plzeň, Czech Republic*
[b] *Institute of Thermomechanics of the ASCR, v.v.i., Dolejškova 5, 182 00 Praha, Czech Republic*

MD simulation is a valuable tool in material science since it provides information on the micromechanics and kinetics of failure in materials, which is often not accessible from experiments. Much attention has been devoted to bcc iron and Fe-Cu system, both in experiments (see e.g. [2, 3, 5]) and theoretical studies [1, 4] because of their importance in structural steel applications, including older reactor ferritic steels. While older experimental observations in the model Fe–Cu dilute alloys brought information concerning bcc Cu nano–particles [3, 5], recent experimental findings show [2] that vacancy–Cu complexes formed by irradiation aggregate into nano–voids where inner surface of the nano–voids is covered by Cu atoms.

Unlike our previous 3D crack simulations [1, 4] where narrow cracks in bcc iron and in Fe-Cu system were studied by means of MD simulations, this paper is devoted to studies of the mechanical response of an atomically blunted cavity uncovered and covered by copper atoms, which was observed in mentioned experiments [2]. Our question is how the copper atoms influence the ductile–brittle behavior at the crack front in comparison with pure bcc iron.

Three different configurations were studied without any periodic boundary conditions: i) the blunted cavity in pure bcc iron; ii) the blunted cavity covered by six copper layers, see fig. 1; iii) the blunted cavity covered by two layers of copper atoms. These studies represent free 3D simulations.

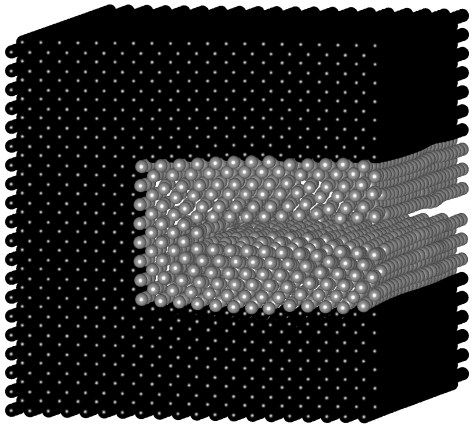

Fig. 1 3D–detail of the configuration.

In the fourth configuration, left corner of the cavity along the crack front was covered by a small Cu inclusion (of the area 8×8 atoms) and these simulations utilized a periodic boundary condition in the x-direction. Here, the total number of atoms is somewhat different, N=98 921 249.

Our MD simulations show that the initially blunted cavity $(001)[010]$ in pure bcc iron at temperature of 0 K is stable after dislocation emission in the inclined systems $\langle111\rangle\{101\}$. Just a small crack deflection after the plastic deformation is observed in the middle of the crystal, well above Griffith level of loading. This ductile behavior is different from our previous 3D simulations with the narrow cavity embedded in the crystal (of the same orientation and geometry) under the same loading conditions at 0 K, where brittle crack initiation was monitored. It indicates

that the brittle→ductile transition can be recalled in bcc iron also at 0 K due to an initial crack blunting, which is theoretically possible also according to continuum predictions.

All the presented results show that the dislocation emission is easier in the Fe-Cu system in comparison with pure bcc iron since the energy needed for dislocation emission in bcc copper is lower than in bcc iron. Here, slip processes are observed both on the inclined $\{101\}$ planes and as well on the oblique $\{112\}$ planes, unlike pure bcc iron, see fig.2. However, stability of the blunted cavities in Fe-Cu systems seems to be weaker in copper region than in pure bcc iron, which could be related to metastable character of bcc copper. Presented results are in a qualitative agreement with our previous MD results, where interaction of Cu nano-particles with an atomically sharp crack $(-110)[110]$ in iron crystals of different orientation was investigated.

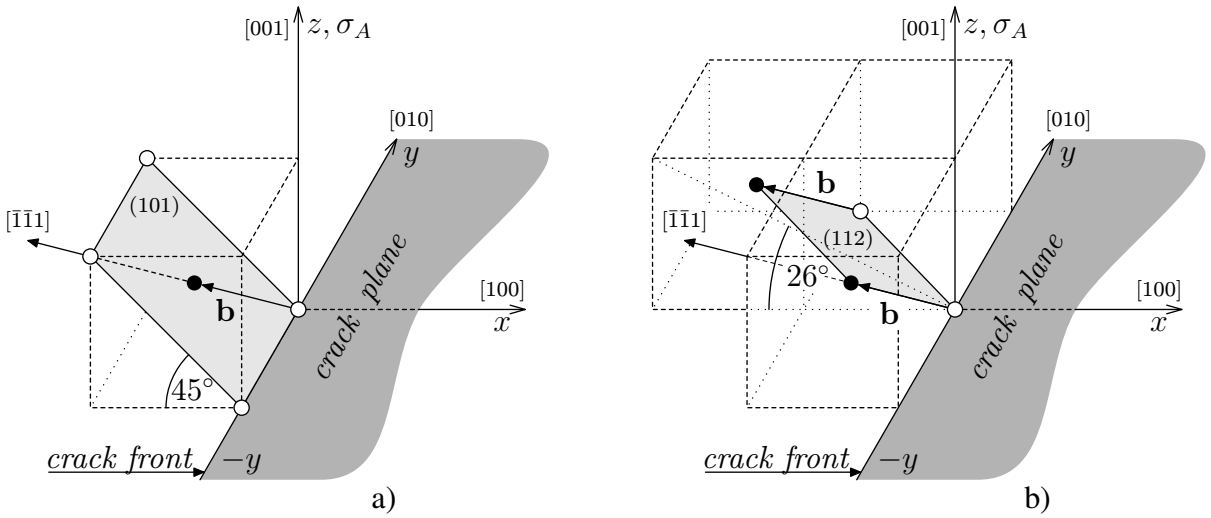

Fig. 2 Scheme of the inclined slip system $\langle 111\rangle\{101\}$ a) and $\langle 111\rangle\{112\}$ b) at the crack front.

Acknowledgments

The work was supported by the Institute Research Plan AV0Z20760514 and by the grants GA CR No 101/07/0789 and GA AS CR KJB200760802. The access to the MetaCentrum clusters provided under the research intent MSM6383917201 is highly appreciated.

References

[1] A. Machová, A. Spielmannová, P. Hora, 3D atomistic simulation of the interaction between a ductile crack and a Cu nanoprecipitate, Modelling Simul. Mater. Sci. Eng. 17 (2009) 035008 19pp.

[2] Y. Nagai, K. Takadate, Z. Tang, H. Ohkubo, H. Sunaga, H. Takizawa, M. Hasegawa, Positron annihilation study of vacancy-solute complex evolution in Fe-based alloys, Physical Review B 67 (2003) 224202-6.

[3] P.J. Othen, M.L. Jenkins, G.D.W. Smith, W.J. Phythian, Transmission electron microscope investigations of the structure of copper precipitates in thermally-aged Fe-Cu and Fe-Cu-Ni, Philosophical Magazine Letters 64 (1991) 383–391.

[4] V. Pelikán, P. Hora, A. Machová, A. Spielmannová, Brittle-ductile behavior in 3D iron crystals, Czechoslovak Journal of Physics 55 (2005) 1245–1260.

[5] W. J. Phythian, A. J. Foreman, C. A. English, J. T..Buswell, M. Herington, K. Roberts, S. Pizzini, The structure and hardening mechanism of copper precipitation in thermally aged or irradiated Fe-Cu and Fe-Cu-Ni model alloys, Proc. 15th Int. Symp. On effects of radiation in Materials, Nashville, Tennessee, ASTM STP, 1990, also in AEA Technology Harwell Report AEA-TRS-2004.