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Ductile–brittle behavior at the (1 1 0)[0 0 1] crack in bcc iron crystals loaded in mode I

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ABSTRACT

Fracture experiments performed at room temperature on four test samples made of Fe–3wt.%Si single crystals with an edge crack (1 1 0)[0 0 1] (crack plane, crack front) showed approximately 45° deflections of the crack from the initial crack plane (1 1 0). This behavior appeared to be independent on loading rate. Fractographic analysis confirmed that the cracks were deviated along {1 0 0} planes and the fracture was accompanied by dislocation slip and by twinning. 3D simulations at 300 K by molecular dynamic technique in bcc iron with edge cracks of equivalent orientation indicated that the crack itself could contribute to understanding of this behavior by three processes: twinning on oblique {1 1 2} planes, which hindered growth of the original crack, and by emission of dislocations on oblique {0 1 1} and {1 2 3} planes, which led to separation of the {1 0 0} planes and might cause decohesion and subsequent cleavage fracture along the mentioned planes.

1. Introduction

Molecular dynamic (MD) techniques rank to the most powerful instruments for modeling of processes at the nanoscale. Numerous calculations proved that it may provide many useful results based on atomistic predictions.

Fe–3 wt.%Si single crystals have been widely used as a model material of ferritic steels mainly for the fact that they exhibit a brittle-to-ductile transition at room temperature. Nevertheless, it has been found that the behavior of this material depends strongly on crystallographic orientation as well as on applied loading rate.

Recent MD simulations (see Spielmannová et al. [1], Prahl et al. [2] and Hora et al. [3]) of crack growth processes in bcc iron have successfully predicted plastic processes observed experimentally in [2], by Marsh et al. [4] and by Spielmannová et al. [5] on Fe–3 wt.%Si single crystals.

Here we present new 3D atomistic and fracture results for crack orientation that was not studied before experimentally. Note that for the studied crack orientation (1 1 0)[0 0 1] only the oblique slip systems to the crack front are available (i.e., there are no inclined slip systems containing the crack front, unlike the orientations studied in [1–5]).

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Nomenclature

2D	two dimensions – plane strain simulations
3D	three dimensions
a	length of the initial edge crack
b	Burgers vector
bcc	body centered cubic
B	thickness of a sample
BLS	block like shear
c	initial half crack opening
d_{hkl}	interplanar distance between planes $\{hkl\}$
E_{loc}	change in the potential energy of an interior atom during BLS simulation
h	time integration step
L	length of a sample
LEFM	linear elastic fracture mechanics
MD	molecular dynamics
KNT	the number of local interactions of individual atoms (coordination number)
SEM	scanning electron microscopy
$u_{\langle 111\rangle}$	shear displacement in the $\langle 111\rangle$ direction
W	width of a sample
σ_A	applied tension stress
τ	shear stress
τ_{disl}	stress barrier for dislocation emission
τ_{twin}	stress barrier for twin generation
γ_{us}	unstable stacking energy

2. Experiments

Four rectangular test samples SEN (single edge notched) were cut from a cylindrical Fe–3 wt.%Si single crystal whose main axis was oriented along the [1 1 0] direction (Fig. 1). The single crystal was produced by the method of floating-zone melting at the Institute of Physics, Academy of Sciences of the Czech Republic (AS CR). The nominal dimensions of the test samples were as follows: length L = 52 mm, width W = 10 mm, and thickness B = 2 mm. The initial 3 mm long notch was cut by an electrospark machine using a Mo wire of 50 μm thickness. The ratio between the notch length and the radius of curvature of the notch a/c exceeded 30, which indicated that the notch could be described by means of linear elastic fracture mechanics (LEFM) [6].

Tensile tests have been carried out on deformation machine INSTRON 1195/58R controlled by PC at the Institute of Thermomechanics, AS CR. The test samples were fixed in special jaws ensuring only mode I loading, as well as constant displacement. The active part of the test samples was approximately 28 mm in all cases. Four different loading rates (from v_E = 0.25–2 mm/min) were used. All tests were performed at room temperature and normal conditions. Time, force, and crosshead dis-

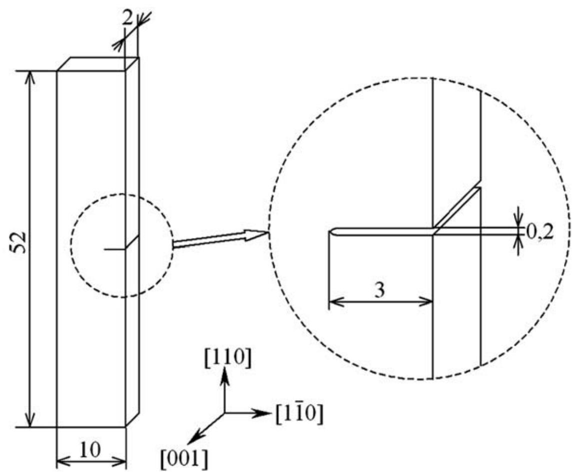

Fig. 1. Dimensions (mm) and crystallographic orientation of SEN test specimens.