Materials Characterization 58 (2007) 892 – 900

MATERIALS CHARACTERIZATION

Influence of crack orientation on the ductile–brittle behavior in Fe–3 wt.% Si single crystals

Alena Spielmannová [a,b,*], Michal Landa [a], Anna Machová [a], Petr Haušild [b], Pavel Lejček [c]

[a] Institute of Thermomechanics AS CR, Dolejškova 5, 18200 Prague 8, Czech Republic
[b] Department of Materials, Faculty of Nuclear Science and Physical Engineering, CTU, Trojanova 13, 12000 Prague 2, Czech Republic
[c] Institute of Physics AS CR, Na Slovance 2, 18221 Prague 8, Czech Republic

Received 26 July 2006; received in revised form 21 August 2006; accepted 2 September 2006

Abstract

In this paper we present experimental results from fracture tests performed at room temperature on bcc iron-silicon single crystals with edge cracks of two different orientations (001)[110] and (−110)[110]. The cracks were loaded under mode I. The fracture toughness and acoustic emission response were measured, and a fractographic analysis obtained via scanning electron microscopy was carried out. Experimental results confirm the basic predictions pertaining to the influence of crack orientation on crack stability from continuum modeling and molecular dynamic simulations in bcc iron.

Keywords: bcc iron; Fracture; Experiments

1. Introduction

Due to fundamental structural applications, the ductile versus brittle response of bcc iron and iron-based materials is often studied experimentally [1–9] as well as theoretically via continuum models [10–13] and atomistic simulations [14–17]. Atomistic simulations use an independent failure criterion given by the range of nonlinear interatomic forces. Namely, simulations by a molecular dynamic (MD) technique enable one to investigate even fast microscopic processes arising at the crack front, e.g. generation of twins, dislocations or microcracks. Generation of defects in MD simulations is a spontaneous process controlled solely by the interatomic forces and external conditions.

Previous continuum analyses and MD simulations [18–21] predict that crack behavior in bcc iron loaded in mode I depends strongly on the mutual orientation of the crack and available slip systems. MD simulations [19,21] show that the crack (001)[110] (crack plane/crack front) is not stable if the inclined slip systems $\langle 111\rangle\{112\}$ are oriented in the so-called “easy” twinning direction. Crack growth in this orientation is either brittle or accompanied by twinning (at low temperatures or higher loading rates). Twinning at the crack front does not lead to crack blunting and enables further crack growth. MD simulations [18,20,21] also indicate that the crack $(\bar{1}10)[110]$ with inclined slip systems $\langle 111\rangle\{112\}$ oriented in the “hard” anti-

* Corresponding author. Institute of Thermomechanics AS CR, Dolejškova 5, 18200 Prague 8, Czech Republic. Tel.: +420 266053023.
E-mail address: spielman@it.cas.cz (A. Spielmannová).

1044-5803/$ - see front matter © 2006 Elsevier Inc. All rights reserved.
doi:10.1016/j.matchar.2006.09.001

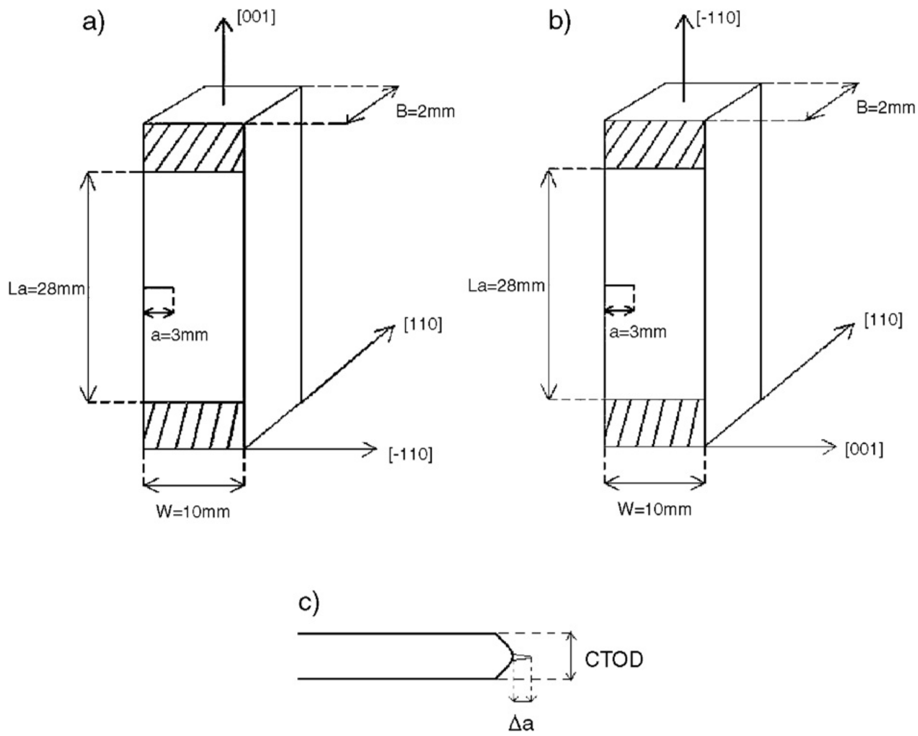

Fig. 1. Schematic view and crystallography of the samples. (a) Sample with edge narrow notch on (001) planes, (b) sample with edge narrow notch on $(\bar{1}10)$ planes, (c) crack tip opening displacement (CTOD) and crack increment Δa.

twinning direction is much more stable, since the crack emits complete dislocations, leading to crack tip blunting.

In this paper we present the results of fracture tests on single crystals of α-Fe (3 wt.% Si) with a very narrow edge notch (an artificial pre-existing crack) of the type (001)and $(\bar{1}10)$[110], respectively. Both types of edge cracks in our experiments were loaded under mode I at room temperature (25 °C). Since our previous experiments [4,9] with the crack orientation (001)[110] have indicated that the brittle–ductile transition at room temperature lies in the region of higher loading rates (V_E=1–5 mm/min), here we are focused on the "transition" region in loading rates. New experimental results on the $(\bar{1}10)$[110] crack orientation are presented in this paper.

2. Experiments

Rod-like single crystals of a Fe–3wt.% Si alloy (diameter of 12 mm; length of 60 mm) with the axis oriented either in the ⟨001⟩ direction or in the ⟨110⟩ direction were grown by the floating zone melting technique at the Institute of Physics, Academy of Sciences of the Czech Republic (ASCR) [22]. A molten zone was established by focusing a 360 kHz induction heating zone in a hydrogen atmosphere and moving it along the material axis at a rate of 10 mm/h. After determining the crystallographic orientation via an X-ray Laue back-scattering technique, rectangular samples of length L of about 52 mm, width W of about 10 mm, and thickness B of about 2 mm were prepared by electrospark cutting. The shape and crystallography of the two types of the samples are schematically shown in Fig. 1a,b. The deformed layer was removed by grinding and by chemical polishing in dilute mixture of HF and H_2O_2. After this procedure, a narrow edge notch of the length a of about 3 mm was electrospark cut using a thin molybdenum wire of diameter of 50 μm. After cutting, the initial crack opening was about $2c \sim 0.08$–0.21 mm.

Table 1
Samples with crack orientation (001)[110] (dimensions are given in mm)

No.	L	W	B	a	c	a/c	a/W
10	53.32	10.25	2.11	2.95	0.085	34.7	0.29
11	53.37	10.22	2.07	2.99	0.080	37.4	0.29
12	53.15	10.22	2.16	2.88	0.105	27.4	0.28
13	51.68	9.6	2	3.27	0.075	43.6	0.34