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Citation	Transactions of JWRI. 39(2) p.238-p.240
Issue Date	2010-12
oaire:version	VoR
URL	https://doi.org/10.18910/11283
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Preliminary numerical research of microstructural fracture behavior in metal by using interface element[†]

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KEY WORDS: (Interface element) (Grain orientation) (Grain boundary) (Finite element method) (Stress concentration)

1. Introduction

Recently, super high strength steel has been developed by controlling its microstructure precisely and this steel has been widely used in various fields. Although there have been various experimental studies about fracture behavior of the high strength steel, its microstructural deformations have not been revealed because only the deformation of grain has been modeled in the conventional finite element method. The authors have developed the interface element in order to model the interfacial deformation such as crack opening, crack propagation and interfacial sliding [1]. In this research, the interface element was employed for modeling the deformation of grain boundary and the microstructural fracture behavior was examined by using the finite element method with the interface element. Namely, the anisotropic deformation of grain due to grain orientation was modeled by the ordinary finite element and the opening and slipping at grain boundary was demonstrated by the interface element where the effect of grain orientation on the mechanical property at the grain boundary was taken into account as the preliminary numerical examination. By using two dimensional microstructure obtained through Voronoi tessellations, the influence of grain orientation on the microstructural fracture behavior was investigated

2. Analysis Method

Model for analysis

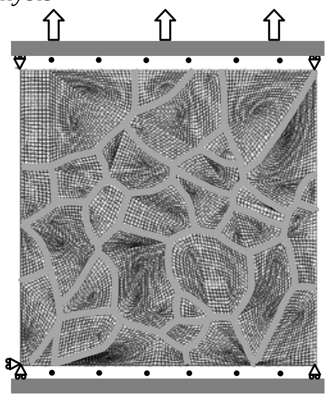

Fig. 1 Finite element model for analysis.

Two dimensional ideal microstructure of steel was created by using Voronoi tessellations and **Fig.1** shows finite element model based on this microstructure. This model contains 30 grains, whose orientations are varied. In order to demonstrate the interfacial deformation, the interface elements were arranged along the grain boundaries.

Interface element

Essentially, the interface element is the distributed nonlinear spring existing between surfaces forming the interface or the potential crack surfaces. The interaction between surfaces is characterized by a potential function that involves the surface energy γ, the shape parameter N and the scale parameter r_0. In order to describe both the opening and sliding deformations at the grain boundary, the combined potential function was employed in this research [1]. The opening and shear stresses to the displacement δ could be described as the following equations, and these relationships are shown in **Fig. 2**.

$$\sigma = \frac{4\gamma N}{r_0}\left\{\left(\frac{r_0}{r_0+\delta}\right)^{N+1} - \left(\frac{r_0}{r_0+\delta}\right)^{2N+1}\right\} \tag{1}$$

$$\tau = \frac{4\sqrt{A}\gamma N}{r_0}\left\{\left(\frac{r_0}{r_0+\delta}\right)^{N+1} - \left(\frac{r_0}{r_0+\delta}\right)^{2N+1}\right\} \tag{2}$$

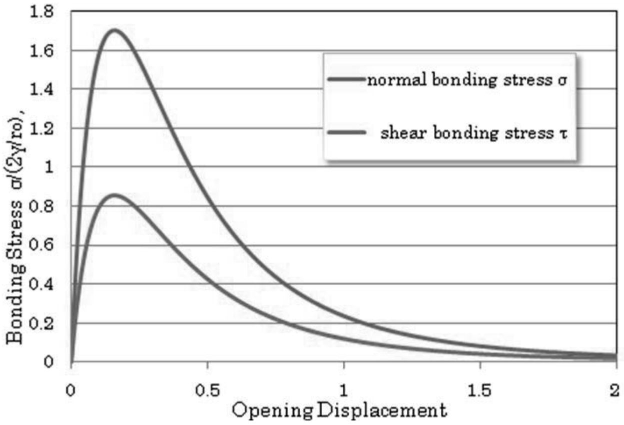

Fig. 2 Opening and shear stresses related to displacement.

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† Received on 30 September 2010

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Transactions of JWRI is published by Joining and Welding Research Institute, Osaka University, Ibaraki, Osaka 567-0047, Japan

Table 1 Stiffness of hexagonal crystal for *a*-Fe.

hexagonal crystal	$(10^{-11}Pa^{-1})$		
	S_{11}	S_{12}	S_{44}
	0.80	−0.28	0.86

The parameters involving the above equations were determined for demonstrating α-Fe fracture behavior. Namely, the surface energy γ and the shape parameter N were assumed to 2.0 N/mm and 4, respectively. The scale parameter r_0 is the property related to maximum bonding and sliding stresses ($\sigma_{\max}$ and $\tau_{\max}$), and was determined according to the misorientation angle between neighbor grains as described in the following section. Also, the interaction parameter A which indicates the ratio σ to τ is included in Eq. (2).

Anisotropy in grain

The properties of each grain in metal materials have anisotropy due to the direction of grain growth. In order to demonstrate the microstructural deformation precisely, the anisotropy has to be taken into account and was assumed by changing the elastic moduli of each directions (E_{11}, E_{22} and G_{12}). The material studied in this research was α-Fe which has hexagonal crystal lattice, and target plane was assumed to (110) plane which contains only tilt boundaries not twist boundaries. Table 1 shows the stiffness of hexagonal crystal for α-Fe [2], and the elastic moduli in anisotropic grain were determined according to the direction of the target plane. Namely, the moduli of each direction in (110) plane (E_{11}, E_{22} and G_{12}) were assumed to 125.0, 210.5 and 66.20 GPa, respectively.

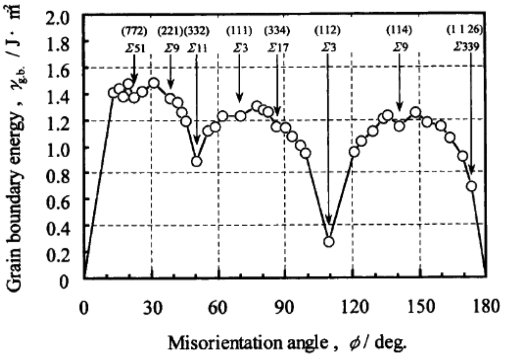


Fig. 3 Relationship between boundary fracture stress and misorientation angle.

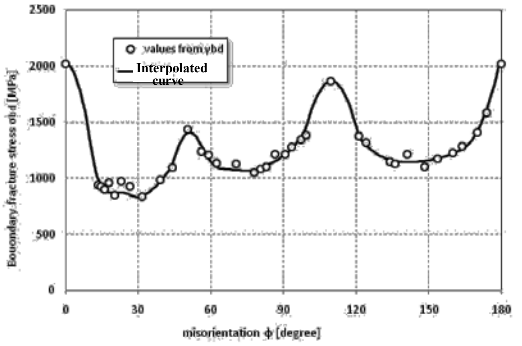
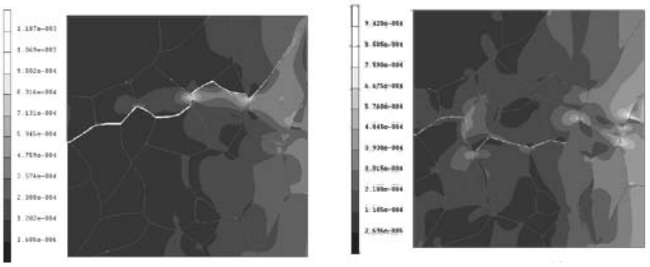


Fig. 4 Relationship between boundary fracture stress and misorientation angle.



(a) Isotropic model (b) Anisotropic model

Fig. 5 von Mises stress distributions

Anisotropy at grain boundary

Generally, the intergranular fracture is caused by crack opening and slipping at grain boundaries. The interface element can demonstrate such deformations by employing the interaction parameter A in Eq. (2). In the case with a low value of parameter A, the interfacial slipping easily occurs in comparison with the crack opening at the interface. The parameter A was varied as 1.0, 0.25 and 0.01 in order to examine the influence of difference between opening and shear strength on the microstructural fracture behavior.

The grain boundary can be regarded as disorder of atoms between neighbor grains. So, it can be assumed that the fracture strength at grain boundary would be related to the boundary energy, which could be determined by the atomic disorder at the boundary. There have been many researches about the symmetric tilt boundary, and various boundary energies in different plane were studied by using the molecular dynamic method. Tanaka *et al.* examined <110> boundary energy of molybdenum and revealed that the square of fracture strength σ_{bd} would be linearly proportional to the grain boundary energy γ_{bd} [3]. Since the boundary energy of α-Fe was reported as shown in **Fig. 3** [4], the authors assumed that the boundary fracture stress of α-Fe would follow the relation to misorientation as shown in **Fig. 4**.

3. Results and Discussions

As a preliminary analysis, the influence of anisotropy in grain on fracture behavior of the model shown in Fig. 1 was examined by assuming only the elastic deformation in grain and the anisotropy at grain boundary. **Fig. 5**(a) and (b) show the typical results of isotropic and anisotropic grains in applying 0.624 % strain, respectively. The interaction parameter in Eq. (2) A was assumed as 0.25, which means that the shear sliding stress τ is half of the bonding stress σ. In the isotropic model, the significant difference among grains was not obtained and the stress distribution was almost homogeneous. So, the position of crack propagation was determined by the distribution of boundary fracture stress at the grain assumed. On the other hand, the stress distribution of the anisotropic model was heterogeneous and stresses among grains were very different. This difference was considered to affect the crack propagation process. In addition, the analyses for studying the influence of interaction parameter A and anisotropy at grain boundary were conducted.

4. Conclusion

In order to demonstrate the microstructural fracture behavior in metal, the finite element method with an interface element was developed. The anisotropy in grain and that at grain boundary were modeled by the ordinary finite element and the interface element, respectively. By using this method, the influence of anisotropy in grain and at grain boundary on the microstructural fracture behavior were examined successfully.

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