CALCULATIONS ON GRAIN BOUNDARY AND INTERFACE FRACTURE

Minoru MORI* and Yoichi ISHIDA**
* Institute of Industrial Science, University of Tokyo, Minato, Tokyo 106, Japan
**Department of Material Science, Faculty of Engineering, University of Tokyo, Bunkyo, Tokyo 113, Japan

ABSTRACT

The Fracture path of impurity segregated bcc iron grain boundaries were simulated. The grain boundary structure were calculated by the molecular dynamical method. There founded unit structure centered by impurity atoms. Strong bonds inside the units were estimated with molecular orbital calculations. Fracture path of P segregated grain boundary was between those units to be considered as weaker bonds. Same method were adopted to the metal/ceramic interface.

Introduction

Grain boundary embrittlement due to segregation is a important probleme specially in steels. Since the fracture process is veryfast, it is difficult to observe the phenomenon in atomic scale. Computer Simulationis the only way to clear thi s mechanism. The segregated grain boundary structures have been simulated using the central force potentials(1-5). Briant and Messmer(6-9) have claculated the molecular orbitals by the self consistent $X\alpha$ scattered wave method. A tetrahedron structure was chosen the atomic configuration as a model of grain boundary structure. Local density of state type calculation showed the strong bonds inside the segregated units and weaker bonds outside the units(10-12).

The grain boundary structures were calculated by MD calculations and its bonds are estimated by SCF-$X\alpha$ calculations.

Molecular dymnamical calculation is adopeted to fracture simulation. Same method are adopted to interface fracture.

Calculations

Calculation methods for segregated grain boundary structures are molecular dynamical technique using Morse type potentials.

$$
\begin{aligned}
V(r) &= A\{\exp[-2\alpha(r-r_0)] - 2\exp[-\alpha(r-r_0)]\} && r < r_o \\
&= A\{\exp[-2\alpha(r-r_0)] - 2\exp[-\alpha(r-r_0)]\} \\
&\quad \times \left[3\left(\frac{r_2-r}{r_1-r_0}\right)^4 - 8\left(\frac{r_1-r}{r_1-r_0}\right)^3 + 6\left(\frac{r_1-r}{r_1-r_0}\right)^2\right] && r_0 < r < r_1 \\
&= 0 && r > r_1,
\end{aligned}
$$

Used parameters are shown in the Table 1. The structures of P or B segregated and non-segregated $\Sigma = 5$ and $\Sigma = 9$ bcc iron grain boundariesare calculated. SCF-$X\alpha$ calculations are performed using the calculated structure of $\Sigma = 5$.

The fracture calculation are simulated using calculated $\Sigma = 5$ structures with notch. Model calculations of Metal/ceramic interfaces are performed. In this case, metal is modeled as a bcc lattice and ceramic is a CsCl structure. Potential for metal is the same as Fe and ceramic potential is artificially chosen

to be the same type but several times stiffer.

Table 1
Morse potential parameters used for the calculation

	A (eV)	r_0 (Å)	αr_0	r_1/r_0
Fe-Fe	0.51	2.58	3.76	1.4
Fe-P	0.848	2.22	3.76	1.4
P-P	0.194	3.35	3.76	1.4

Results and Discussions

Fig. 1 shows the grain boundary structures of bcc iron with or without P atoms. the grain boundary plane is (031) and (114) in the case of $\Sigma=5$ $\Sigma=9$, respectively. The unit structure with P segregated grain boundaries are almost the same in $\Sigma=5$ and $\Sigma=9$. Boron segregated structure of $\Sigma=5$ grain boundary is resembles to non-segregated structure except B atoms are at the center of the prisms at the grain boundary.

Substitutional segregate position such as P atom case tend to have a little distance from a grain boundary plane and the sturucture units centered by segregated atoms tend to place zigzagly. While interstitialtype segregatation case, atom positions are on a grain boundary plane.

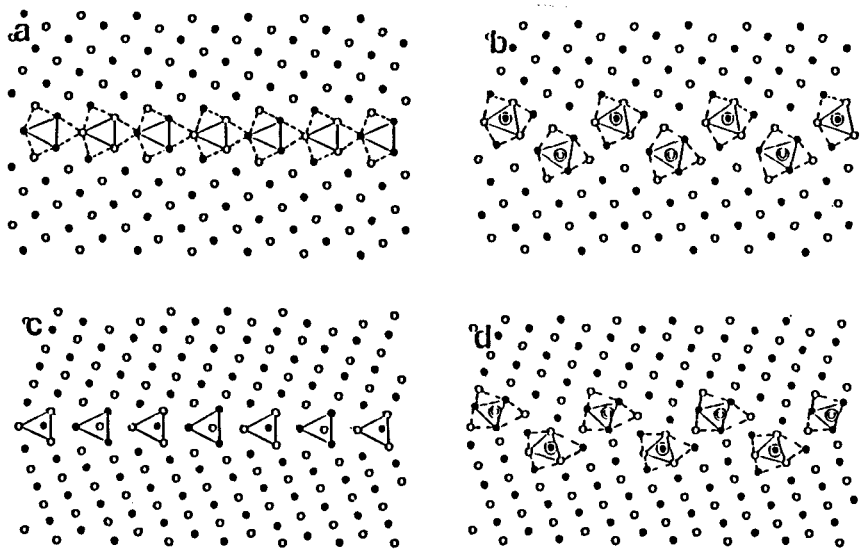


Fig. 1 Grain boundary structures of $\Sigma=5$ (a, b) and $\Sigma=9$ (c, d) coincidence grain boundaries without P (a, c) and with P segregation (b, d). Double circles indicate P atom positions. Black and white circles indicate the different atom planes.

Fig. 2 shows the schematical representation of electron densities at the plane between atomic planes. Both B segregated and P segregated case, their seems strong bonds inside the unit structures and weeker bonds between these structures.

Fe

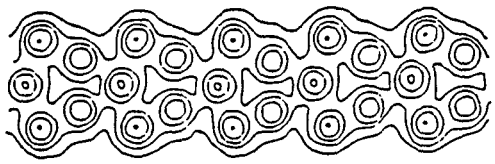
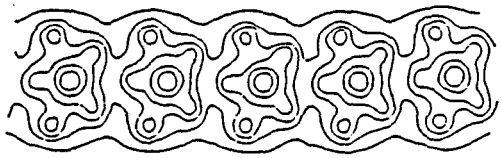


Fig. 2 Periodically arranged electron density at the midplane of atomic planes.

Fe-B



Fe-P

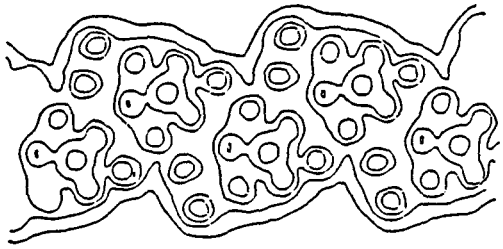


Fig. 3 is the grain boundary structure with tensile stress perpendicular to the grain boundary. The stress applied was $1X10^{3}$ MPa. Initially crack path was set on the grain boundary plane inside the structure unit at the both sides. After the stress was applied the fracture path was along the side of the structure units expected as the weaker bond regionby the molecular orbital calculations.

(a) (b) (c)

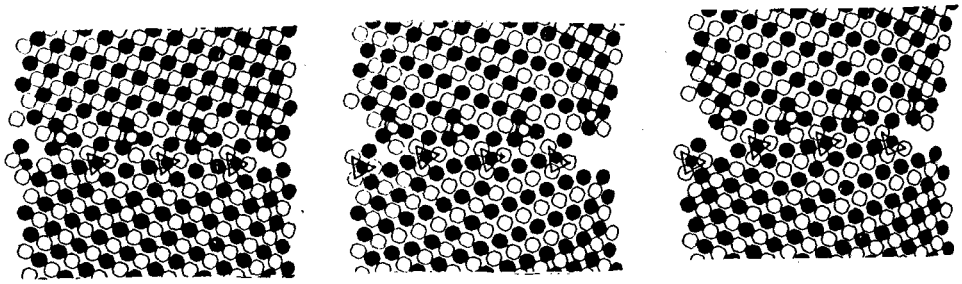


Fig. 3

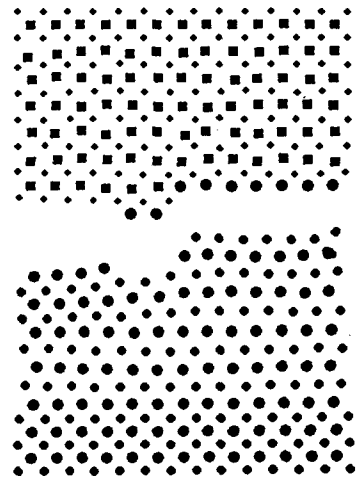
Grain boundary fracture under a tensile stress $1X10^{3}$ MPa in a $\Sigma = 5$ grain boundary. Smaller circles denote P atom positions. Black and white circles indicate the different atom planes. $4X10^{-12}$s after the application of the tensile stress (a), $8X10^{-12}$s (b) and $1.2x10^{-11}$s (c)

In the metal/ceramic interface fracture case, only a model calculation were carried out (Fig. 4). Lower part of Fig. 4 is the modeled metal as a bcc lattice and Morse potential parameters of them are same as iron. Upper part is a modeled ceramic as a Cs-Cl structure larger squares denote aluminium and smaller squares are oxgen. The potential parameter A in this case was twice larger than Fe-Fe case.

In Fig. 4 there was a one atomic ledge at the center of interface. This kind of ledge was observed in the Al_2O_3/Ni deffusion bonded interface. Movement of this structure may affect to decreese thermal strain during colling.

Initial nottch of four lattice was introduced in the model. The deviation of the crack is one atomic layer away from the in terface. This tendency was not influenced by the initial notch length or the ledge exsostance.

Fig. 4 Mdeled metal/ceramic interface fracture. Upper part denote ceramic and lower part is metal.



REFERENCE

(1)M. Hashimoto, Y. Ishida, R. Yamamoto and M. Doyama; Acta Metall., 32(1984), 1

(2)M. J. Weins and J. P. Weines; J. de Physique, 36 C4(1975), 97

(3)S. Nicholas; Scripta metall., 15(1981), 423

(4)A. P. sutton and V. Vitek; Acta Metall., 30(1982), 2011

(5)Y. Ishida, M. Mori and M. Hashimoto; Surface Science, 144(1984), 253

(6)C. L. Briant and R. P. Messmer; Phil. Mag., B42(1980), 569

(7)R. P. Messmer and R. P. Briant; Acta Metall., 30(1982), 457

(8)C. L. Briant and R. P. Messmer; Acta Metall., 30(1982), 1811

(9)C. L. Briant and R. P. Messmer; Acta Metall., 32(1984), 2043

(10)M. Hashimoto, Y. Ishida, S. Wakayama, R. Yamamoto, M. Doyama and T. Fujiwara; Acta Metall., 32(1984), 13

(11)M. Hashimoto, Y. Ishida, R. Yamamoto, M. Doyama and T. Fujiwara; Surface Science, 144(1984), 182

(12)M. Mori and Y. Ishida; Proc. of JIMIS-4, 361(1986)