

FIRST PRINCIPLES MOLECULAR DYNAMICS CALCULATION ON THE TENSILE STRENGTH OF Al GRAIN BOUNDARY

Guang-Hong LU¹, Masanori KOHYAMA² and Ryoichi YAMAMOTO¹

¹ Institute of Industrial Science, University of Tokyo, 7-22-1 Roppongi,
Minato-ku, Tokyo 106-8558, Japan

² Department of Materials Physics, Osaka National Research Institute, AIST,
1-8-31 Midorigaoka, Ikedashi, Osaka 563-8577, Japan

ABSTRACT

The *ab initio* tensile test has been applied to Al $\Sigma 9(2\bar{2}1)/[110]$ tilt grain boundary by first principles plane-wave pseudopotential method based on density functional theory with local density approximation. Stress-strain relation shows that the maximum stress of the Al $\Sigma 9$ grain boundary is 9.9GPa at the strain of 28%. The changes of the charge density and the bond length indicate that the bonds at the boundary break first.

KEYWORDS

first principles, tensile strength, aluminum, grain boundary

INTRODUCTION

It is possible now to investigate the strength and mechanical behavior of defect, interface and grain boundary directly through first principles calculations on large supercell, using the first principles molecular dynamics method[1-3]. Deyirmenjian et al.[4] first performed *ab initio* tensile test on aluminum with atomic-scale void. Kohyama[5] performed the calculation of the tensile strength and fracture of a tilt grain boundary in

cubic SiC by the same scheme. In both calculations the supercell is extended by a small increment and then relaxed to its ground-state configuration using the first principles pseudopotential method. The total energy and the average stress are obtained for each level of extension. By iterating this cycle, the maximum stress σ_{\max} can be obtained at the corresponding strain ε_{\max} . This should correspond to a real tensile test at zero temperature.

In this paper, we perform an *ab initio* tensile test on Al $\Sigma 9$ grain boundary in order to investigate how aluminum containing the grain boundary fails as it is pulled apart at zero temperature.

COMPUTATIONAL METHOD

The unit cell is constructed as shown in Figure 1. Al $\Sigma 9(2\bar{2}1)/[110]$ tilt grain boundary is formed by rotating grain by 38.94° along the $[110]$ axis, and $(2\bar{2}1)$ is set as the boundary plane. The coincidence site lattice (CSL) unit cell on the boundary plane is defined by $\frac{3\sqrt{2}}{2}a_0[1\bar{1}4]$ and $\frac{\sqrt{2}}{2}a_0[110]$. The size in the $[110]$ direction is set twice that of the CSL, i.e. $\sqrt{2}a_0$. In the $[2\bar{2}1]$ direction two symmetric boundaries are introduced to make the periodicity. The distance between the grains is determined by that the atom density in boundary is the same as that of the unit cell in the ref.[6].

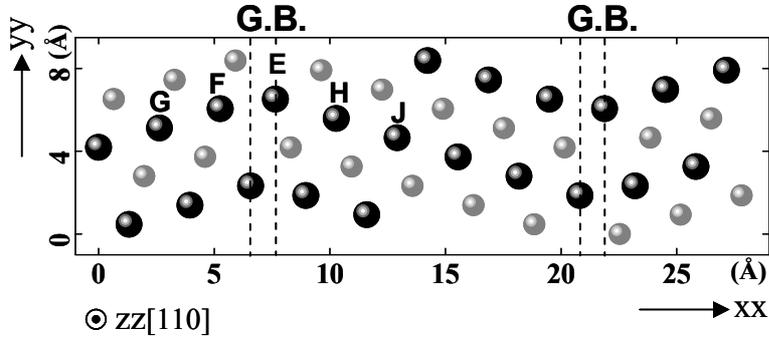


Figure 1: The cross section of $zz[110]$ direction of the unit cell, Al $\Sigma 9(2-21)/[110]$ tilt grain boundary. There are four (110) atomic layers, A, B, C and D. The length of three sides are 28.469\AA (xx), 8.379\AA (yy) and 5.586\AA (zz), respectively. There are 84 atoms in the unit cell. F, G, E, H and J are the atom positions of B layer marked for later discussions. The dark-grey spheres indicate the atoms of B (or D) layer in the unit cell. The light-grey spheres indicate the atoms of A (or C) layer in the unit cell.

Total energy, atomic forces and averaged stresses can be obtained quantitatively[7] by the *ab initio* plane-wave pseudopotential method[8] based on density functional theory (DFT)[9-10] with local density approximation (LDA)[11]. The pseudopotentials of Al is constructed[12] using Troullier-Martins scheme[13]. The separable form by Kleinman and Bylander[14] with the p orbital as the local component is used. The lattice parameters calculated by the pseudopotentials are 3.95\AA for fcc Al, which is in good agreement with the corresponding experimental value of 4.02\AA (0K)[15]. The electronic ground state is

obtained efficiently using the conjugate-gradient technique proposed by Bylander, Kleinman and Lee[16] with the Kerker mixing scheme[17]. The plane wave energy cutoff is 15Ry, and 32 k points in the Brillouin zone are used. The electronic structure is determined by a real space grid of $256 \times 64 \times 32$ points.

In the tensile test, a uniaxial tensile strain is introduced into the stable configuration. The supercell is stretched by a small increment in xx direction that is normal to the boundary plane. The length of the yy and zz direction is fixed in order to save the computational time. This means Poisson's ratio has not been considered. The atomic positions are changed by uniform scaling. Then all the atoms are relaxed according to the Hellman-Feynman forces until all the forces are less than $0.15\text{eV}/\text{\AA}$. The total energy and stress tensor are calculated. This cycle is iterated until the stress reaches the maximum value. During the tensile test, the symmetric property of the system is naturally preserved.

RESULTS AND DISCUSSIONS

Figure 2 shows the change of the total energy with the increase of the tensile strain. It can be seen that the total energy decreases before the strain of 1%. After the strain of 1%, the total energy increases. This should be due to the boundary expansion after the initial relaxation (see Figure 3). Therefore there exists the compressive residual stress in the unit cell. When the unit cell is stretched, the

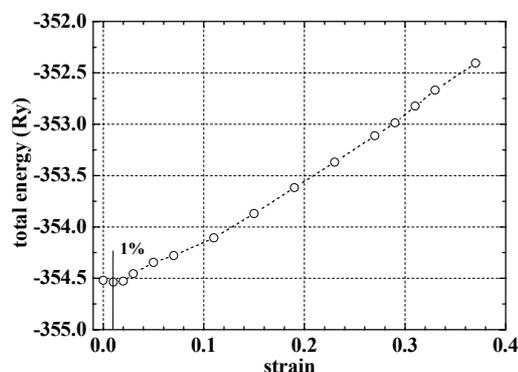


Figure 2: Total energy change with the tensile strain in the *ab initio* tensile test of the Al $\Sigma 9$ grain boundary

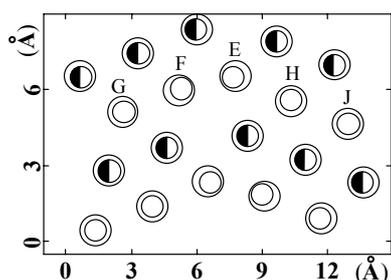


Figure 3: The relaxed configuration of the left half part of layer B and A in the unit cell. G, F, E, H and J correspond to the atoms marked in Figure 1. The atom positions before the relaxation are represented by the smaller circles, in which the unfilled and the half-filled ones represent the atom positions of B and A layer, respectively. The bigger circles indicate the atom positions after the relaxation.

residual stress will be relaxed at first, thus the system becomes stable and the total energy becomes lower.

The stress-strain curves of Al grain boundary are shown in Figure 4. Only those of $xx([2\bar{2}1])$, $yy([1\bar{1}4])$, $zz([110])$ direction are plotted. The stress in other directions is so small to be ignored. Figure 4(a) shows the stress-strain relation in xx direction. At the strain of 3%, the stress on the unit cell becomes positive, thus 3% is set as zero strain in the stress-strain curve. It is shown that the stress increases with the increase of the strain.

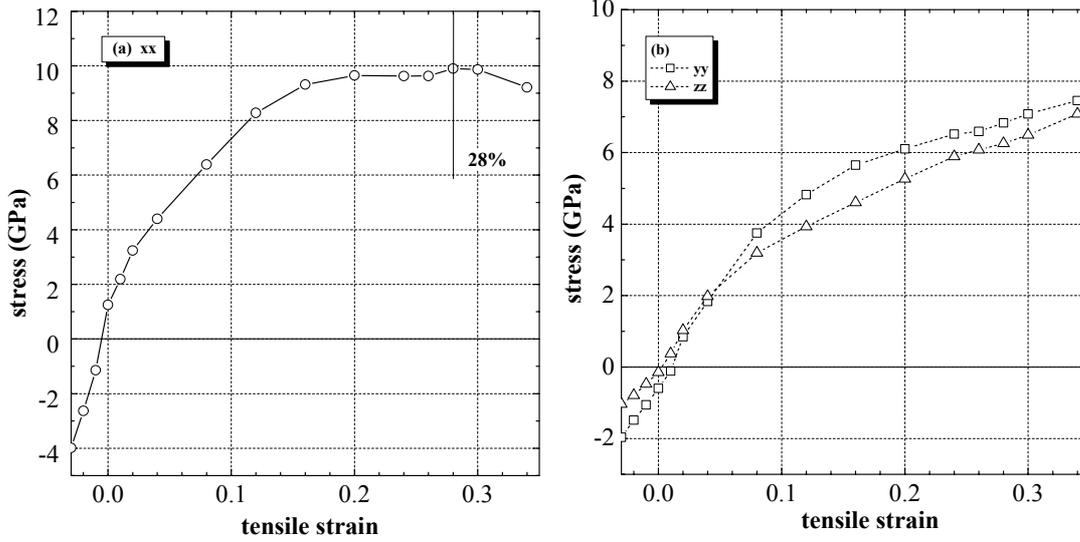


Figure 4: stress-strain relations of Al $\Sigma 9$ grain boundary
(a) xx direction (b) yy, zz directions

At the strain of 28%, the stress is maximum, about 9.9GPa. After the strain of 28%, the stress decreases.

In real case, the size of yy, zz direction should decrease when the unit cell is stretched according to xx direction. Because the Poisson's ratio is not considered in this tensile test in order to save the computational time, there exists the stress also in the yy, zz directions (see Figure 4(b)).

TABLE 1

THE MAXIMUM STRESS σ_{\max} AND THE CORRESPONDING STRAIN ε_{\max}

	ε_{\max}	σ_{\max} (GPa)
Al boundary	28%	9.9
fcc Al [001] ^a	20%	11
experiment ^b	2.9%	2.25

^a ref.[4] ^b ref.[18]

Table 1 shows the maximum stress σ_{\max} and the corresponding strain ε_{\max} of Al single crystal by both the experiment and the calculation. The maximum stress of Al boundary in our calculation is a bit lower than that of [001] direction of Al single crystal calculated by Deyirmenjian et al.[4], i.e., 11GPa. This means Al grain boundary still bonds strongly. The maximum stress of single crystal of Al fiber tested by Gane[18] is about 2.25GPa, much smaller than that by this calculation. This should be due to:

1. Poisson's ratio is not considered in the calculation. The presence of Poisson's ratio generally decreases the maximum stress.

2. Dislocation is not considered in the calculation. In real crystals, the motion of dislocation usually results in a reduction in strength.

Furthermore, the changes of the charge density and the bond length with the increase

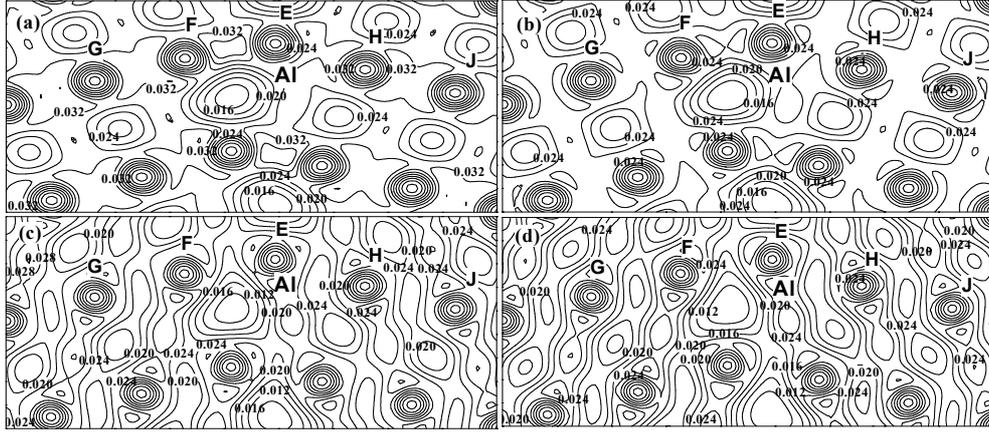


Figure 5: The charge density distribution of the left half part of the B layer in the unit cell (a) no strain (b) 2% (c) 20% (d) 28%

of the strain are investigated. Figure 5 shows the charge density with no strain, and at the strain of 2%, 20% and 28%, respectively, in the left half part of the B layer of the unit cell. It can be indicated that the charge density becomes lower with the increase of the strain. The charge density with no strain between EF bond is above $0.036/\text{a.u.}^3$, and near $0.032/\text{a.u.}^3$ at the strain of 2%. Both values are the highest ones comparing to that between other bonds, such as FG, EH, HJ bonds. However, at the strain of 23% the charge density between EF bond is below $0.024/\text{a.u.}^3$, and at the strain of 28% corresponding to the maximum stress, the charge density is below $0.016/\text{a.u.}^3$. Both values are the lowest ones comparing to that between other bonds such as FG, EH, HJ bonds. Therefore it has high possibility that EF bond breaks first.

Figure 6 shows FG, EF, EH, HJ bond-length changes during the tensile test. The vertical axis is set as:

$$\frac{l - l_{Al}}{l_{Al}} \times 100 \quad (1)$$

Where l is the bond length of FG, EF, EH or HJ and l_{Al} is the bond length of fcc-Al, i.e. 2.80\AA from our calculation. It is clear that the bond length increases with the increase of the strain. At first the four bonds increase in the same rate. However EF bond length increases more rapidly from the strain of 16%. On the contrary, FG bond length increase becomes slower. Therefore it can be concluded that EF bond breaks first with the increase of the strain. Notice EF bond locates just at the boundary, therefore the bond at the boundary breaks first.

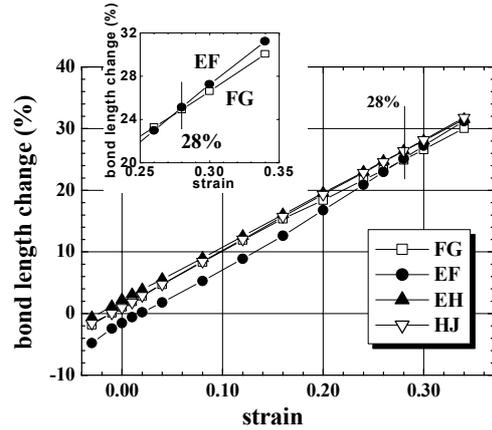


Figure 6: FG, EF, EH, HJ (B layer in the unit cell) bond length changes during the *ab initio* tensile test

CONCLUSIONS

The *Ab initio* tensile test has been applied to Al grain boundary for the first time by first principles molecular dynamics method. The maximum stress is 9.9GPa for Al Σ 9 grain boundary at the strain of 28%. This is a bit lower than the maximum stress (11GPa) of [001] direction of Al single crystal calculated by Deyirmenjian et al., which means Al grain boundary still bonds strongly. Because the Poisson's ratio and the dislocation are not considered in this calculation, the maximum stress of Al boundary is much higher than that of single crystal of Al fiber (2.25GPa). The changes of the charge density and the bond length indicate that the bonds at the boundary break first.

ACKNOWLEDGEMENTS

The research is supported by the Science and Technology Agency of Japan as the joint research with National Research Institute for Metals (NRIM), and also partly by the Science and Technology Promotion of Japan.

REFERENCES

1. Car, R. and Parrinello, M. (1985) Phys. Rev. Lett., **55**, 2471
2. Teter, M. P., Payne, M. C. and Allan, D. C. (1989) Phys. Rev. B, **40**, 12255
3. Payne, M. C., Teter, M. P., Allan, D. C., Arias, T. A. and Joannopoulos, J. S. (1992) Rev. Mod. Phys., **64**, 1045
4. Deyirmenjian, V. B., Heine, V., Payne, M. C., Milman, V., Lynden-Bell, R. M. and Finnis, M. W. (1995) Phys. Rev. B, **52**, 15191
5. Kohyama, M. (1999) Phil. Mag. Lett., **79**, 659
6. Mills, M.J., and Daw, M.S. (1990) Mat. Res. Soc. Symp. Proc., **183**, 15
7. Nielsen O. H. and Martin R. M. (1985) Phys. Rev. B, **32**, 3780; (1987) **35**, 9308
8. Pickett, W.E. (1989) Comput. Phys. Rep., **9**, 115
9. Hohenber, G P. and Kohn, W. (1964) Phys. Rev. B, **136**, 864
10. Kohn, W., and Sham, L.J. (1965) Phys. Rev. A, **140**, 1133
11. Perdew, J. P., and Zunger, A. (1981) Phys. Rev. B, **23**, 5048
12. Hoekstra, J., and Kohyama, M. (1998) Phys. Rev. B, **57**, 2334
13. Troullier, N., and Martins, J. L. (1991) Phys. Rev. B, **43**, 1993
14. Kleinman, L., and Bylander, S. M. (1982) Phys. Rev. Lett., **48**, 1425
15. Lam, P. K., and Cohen, M. L. (1981) Phys. Rev. B, **24**, 4224
16. Bylander, D. M., Kleinman, L., and LEE, S. (1990) Phys. Rev. B, **42**, 1394
17. Kerker, G. P. (1981) Phys. Rev. B, **23**, 3082
18. Gane, N. (1970) Proc. Roy. Soc. Lond. A, **317**, 367