OPEN ORBITS IN HIGH-PURITY ALUMINIUM

HIROKI HOSODA, YOSHITAKE UEDA*, YASUHIKO DEGUCHI AND TAKAO KINO*
Department of Physics, Faculty of Education, Ehime University, Bunkyo-cho, Matsuyama 790 Japan
*Laboratory of Crystal Physics, Faculty of Science, Hiroshima University, Kagamiyama, Higashi-Hiroshima 724 Japan

ABSTRACT

The fraction of conduction electrons which participate of the creation of [010] and [110] open orbits in aluminium has been calculated by the 4-OPW method in magnetic fields 0.125 ∿4 T against the inclination angles 0° ∿6° of the field direction from [001]. The results have been compared with the experimental data of magnetoresistance. The fraction increases with the magnetic field. For the [110] open orbit, the inclination angle dependence of the fraction has a peak, and the peak angle increases with the magnetic field. On the other hand, for [010] open orbit, the fraction increases and attains to a nearly constant value at a critical angle which increases with the magnetic field. The peak and critical angles 0.5° calculated for B = 0.125 T consist with the experimental peak angle measured at B = 4 T. This suggests that the gap energy in real crystals is about 6 times larger than that calculated one, and the difference comes from the rounding of Fermi surface due to imperfections in real crystals.

INTRODUCTION

The energy gap between the Fermi surface in the second Brillouin zone and that in the third Brillouin zone in aluminium is very small near the W-point. Conduction electrons can go through the energy gap easily in a high magnetic field. Such a phenomenon is called as "magnetic breakdown". A fraction of electrons participate in open orbits and extended orbits due to the magnetic breakdown, and the magnetoresistance increases. The probability of the occurrence of the magnetic breakdown depends on the position of the Landau levels near the β-orbit to the Fermi level, so the magnetic-breakdown oscillations caused by the creation of these open orbits appear and the period has the same one in de Haas-van Alphen effect.

The magnetic-breakdown oscillations in magnetoresistance in aluminium have been investigated by several workers.[1 ∿ 4] The gap energy is estimated as 45 ∿ 75 meV for open orbits and an extended orbit by a precise experiment using single crystals of zone-refined aluminium.[5] The gap energy is much larger than the gap energy 0 ∿ 9.2 meV calculated in the 4-OPW model, and the difference is explained by the rounding of Fermi surface due to imperfections in real crystals.

When a magnetic field inclines from [001] to [1$\bar{1}$0] and [100] in single crystals with the lengthwise directions of [110] and [010], respectively, the transverse magnetoresistance changes with the inclination angle ψ, a large peak appears at about 0.5° in a magnetic field 4 T, and the peak comes from the creation of open orbits due to the magnetic breakdown.[2 ∿ 5] When a magnetic field inclines over the peak angle, the gap energy with respect to the open orbit increases, and at the same time a plane which includes the open orbit deviates from the Γ-point, so the magnetoresistance decreases. On the other hand, when the direction of the magnetic field approaches to [001], the magnetic breakdown can occur easily not only in the direction along the open orbit but also in the direction that the electrons go away from the open orbit at the β-orbits with respect to the open orbit. Therefore, the creation of the open orbit is suppressed and the magnetoresistance decreases. The probability that the electrons go away from the open orbit depends on the gap energy, so the gap energy is estimated also from the peak angle in the magnetoresistance. Considering the probability that the electrons go away from the open orbit, the fraction of electrons that participate in two kinds of open orbits shown in Fig. 1 were calculated by the 4-OPW method.

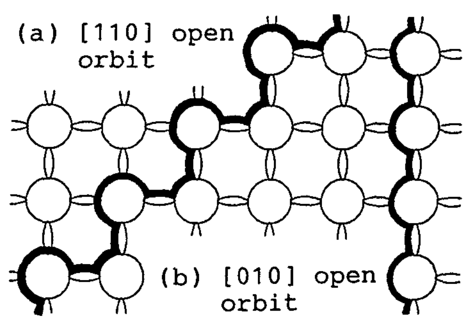

Fig.1 The schematic profile of open orbits in k-space along (a) [110] direction and (b) [010] direction.

METHOD OF CALCULATION

The probability p of the occurrence of the magnetic breakdown is given by the gap energy E_g and a magnetic field B as follows:[1]

$$p = \exp\left(- \frac{m \quad E_g^2}{\hbar \quad e \quad E_F \quad B} \right), \tag{1}$$

where m, e, $\hbar$ and E_F are the effective electronic mass, the electronic charge, the Plank's constant divided by 2π and the Fermi energy, respectively. The electronic rest mass was used for the effective mass in this calculation.

The probability P to create a period of an open orbit in the k-space was calculated from the probabilities p_i and $p_{i'}$ of the occurrence of the magnetic breakdown shown in Fig. 2 as follows. P is proportional to the probability

$$P_i = p_i \times p_{i'} \tag{2}$$

that a conduction electron goes through a β-orbit on the open orbit from the Fermi surface in the second Brillouin zone to that in the next one. On the other hand, at the other β-orbits near the open orbit, P is proportional to the probability P_i^* that a conduction electron does not go from the second zone to the next one, where P_i^* was given as

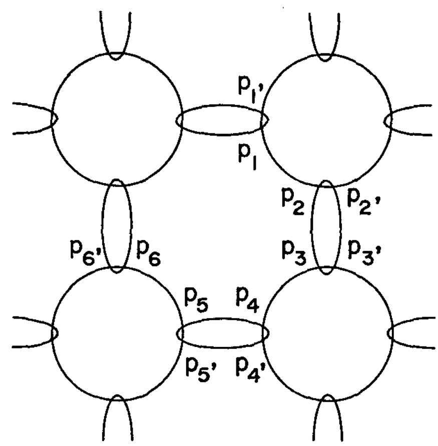

Fig.2 The position where the magnetic breakdown occurs.

$$P_i^* = 1 - p_i + \frac{p_i^2\ (1 - p_{i'})}{1 - (1 - p_i)(1 - p_{i'})} . \tag{3}$$

From relations (2) and (3), P was calculated as

$$P = P_1\ P_2^*\ P_3^* \tag{4}$$

and

$$P = P_1\ P_2^*\ P_3^*\ P_4^*\ P_5^*\ P_6 \tag{5}$$

for the [010] and [110] open orbits, respectively. In order to compare the above results with the magnetoresistance data, the probability $P(k_z)$ per one β-orbit was given as

$$P(k_z) = P \tag{6}$$

and

$$P(k_z) = \sqrt{P} \tag{7}$$

for the [010] and [110] open orbits, respectively. $P(k_z)$ was integrated between the α-orbits shown in Fig. 3 and divided by the distance between these α-orbits. In this way, the fraction R of conduction electrons that participate in the open orbit for the total number of electrons between the α-orbits was calculated against the inclination angle ψ of the magnetic field direction from [001] using the 4-OPW parameter determined by Joss and Monnier.[6]

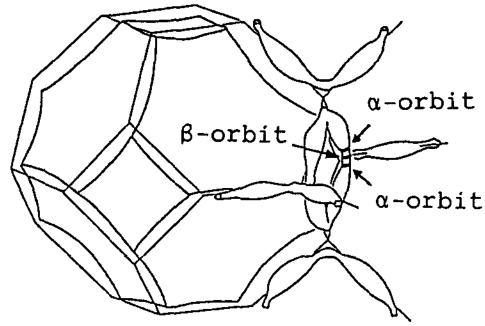

Fig.3 Fermi surface of aluminium.

RESULTS OF CALCULATION

The fraction R of conduction electrons for the [010] open orbit calculated with B = 0.125, 0.25, 0.5, 1, 2 and 4 T are shown in Fig. 4. When the inclination angle ψ increases, R increases and attains to a nearly constant value at a critical angle. The fraction R and the critical angle increases with the magnetic field.

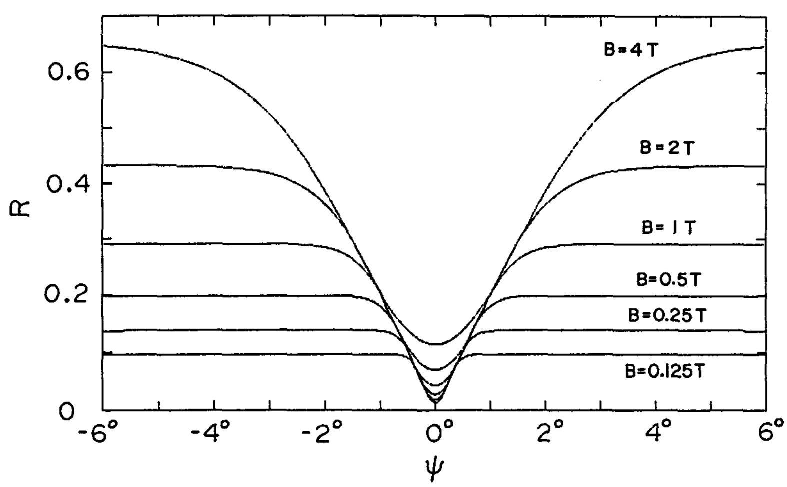

Fig.4 The ψ-dependence of the fraction R of conduction electrons that participate in the [010] open orbit calculated from the 4-OPW model for B = 0.125, 0.25, 0.5, 1, 2 and 4 T.

The fraction R for the [110] open orbit calculated with B = 0.125, 0.25, 0.5, 1, 2 and 4 T are shown in Fig. 5. The ψ-dependence of R has a peak, and the peak angle increases with the magnetic field.

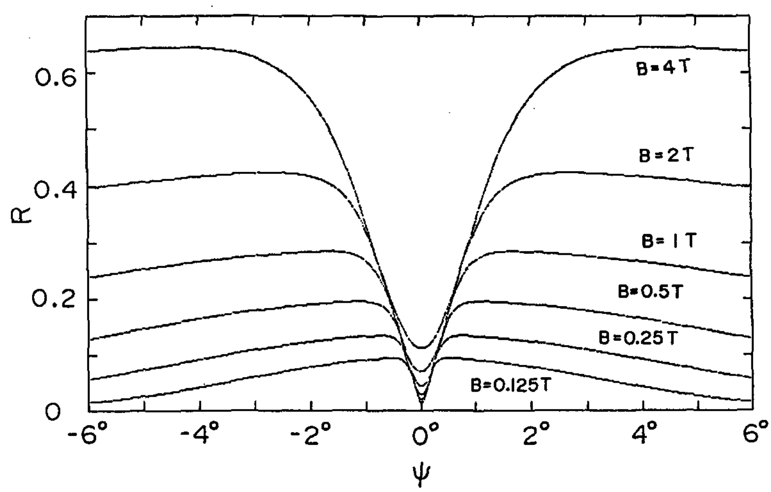

Fig.5 The ψ-dependence of the fraction R of conduction electrons that participate in the [110] open orbit calculated from the 4-OPW model for B = 0.125, 0.25, 0.5, 1, 2 and 4 T.

DISCUSSION

Magnetoresistance of aluminium single crystals measured in a magnetic field 4 T has a large peak around 0.5° of the inclination angle ψ.[2∿5] On the other hand, the calculated value R for the [110] open orbit has a peak around 0.5° for 0.125 T in the magnetic field as seen in Fig. 5. For the [010] open orbit, the contact of the Fermi surfaces in the 4-OPW model prevents the decrease of R, so the critical angle is considered to correspond to the experimental peak angle. Also in this case, the consistency of both angles is well for B = 0.125 T. Therefore, from relation (1), the gap energy in the present specimen is expected to be almost 6 times larger than that calculated in the 4-OPW model.

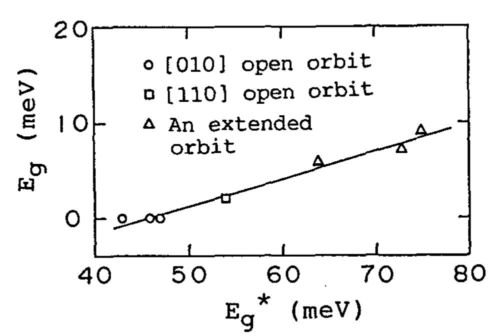

Fig.6 The gap energy calculated in the 4-OPW model against that estimated from the data of magnetic-breakdown oscillations.

Figure 6 compares the gap energy E_g in the 4-OPW model with the experimental one E_g^*.[5] The gap energy E_g^* has a linear relation to E_g as follows:

$$E_g^* = 46\ [\text{meV}] + 3.4 \times E_g \, . \qquad (8)$$

The average value of E_g^* is almost one order of magnitude larger than that of E_g. Using the above relation, the fraction R was calculated for B = 4 T, and the results are shown in Fig. 7. The peak and critical angles for the [110] and [010] open orbits are 0.5° and 0.8°, respectively, which agree with the experimental results.

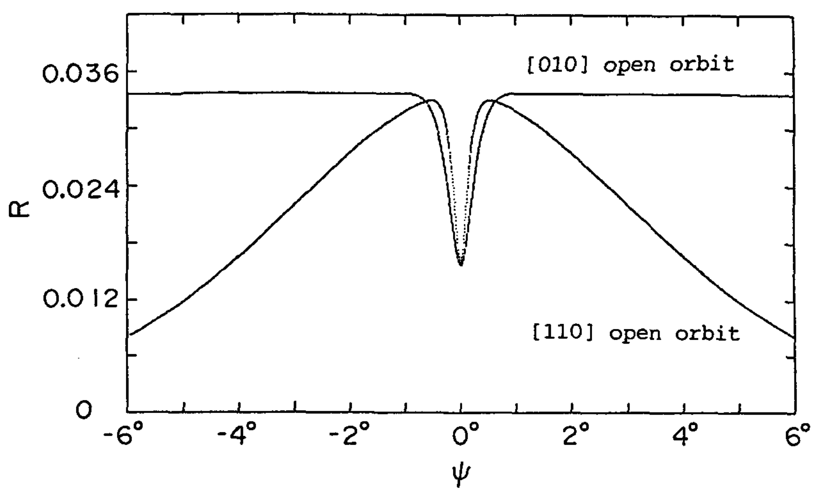

Fig.7 The ψ-dependence of the fraction R of conduction electrons that participate in the [010] and [110] open orbits calculated for B = 4 T using the relation: $E_g^* = 46$ meV + $3.4 \times E_g$.

In conclusion, the gap energy in real crystals is about 6 times larger than that calculated one, and the difference seems to come from the rounding of Fermi surface due to imperfections in real crystals.

REFERENCES

[1] R. J. Balcombe and P. A. Parker: Philos. Mag. 21 (1970) 533.
[2] W. Kesternich and C. Papastaikoudis: J. Phys. F7 (1977) 837.
[3] H. Sato, K. Shimizu and K. Yonemitsu: J. Low Temp. Phys. 35 (1979) 41.
[4] H. Hosoda, Y. Ueda and T. Kino: J. Phys. Soc. Jpn. 56 (1987) 2858.
[5] H. Hosoda: J. Sci. Hiroshima Univ. A55 (1991) 115.
[6] W. Joss and R. Monnier: J. Phys. F10 (1980) 9.