反射高速陽電子回折の理論
Theory of Reflection High-Energy Positron Diffraction for Surface Studies

一宮彪彦 [1]

Ayahiko Ichimiya[1]

[1]*Nagoya University, Furocho, Chikusa-ku, Nagoya 464-8601, Japan.*

*e-mail: ichimiya(at)nagoya-u.jp

Reflection high-energy positron diffraction (RHEPD) is a powerful tool for surface studies. Since crystal potential for positrons is opposite sign of that of electrons, the kinetic energy of positrons decreases in crystals, while that of electrons increases. This means that mean kinetic energy of positrons in a crystal, E, is given as $E = E_0 - eV_0$, where E_0, e and V_0 are incident positron energy, the elementary charge and mean inner potential of the crystal, respectively. Here, $eV_0 > 0$ for positrons. A mean wave number of positrons, k, in the crystal is given as $k = 1.02\ E^{1/2}$ (*in* $Å^{-1}$). In order to satisfy the wave continuity at the surface, we take that

$$k_{0p} = k_p$$

and

$$k_p^2 + k_n^2 = k_{0p}^2 + k_{0n}^2 - 1.05eV_0.$$

Here subscripts p and n means surface parallel and surface normal components, respectively. Then

$$k_n^2 = k_{0n}^2 - 1.05eV_0.$$

When $k_{0n} < 1.02\ (eV_0)^{1/2}$, the surface normal wave number in the crystal becomes imaginary value. At this incident condition positron beams are totally reflected. Using a glancing angle of the incident positron beam, θ, since

$$k_{0n} = k_0 \sin\theta = 1.02\ E_0^{1/2} \sin\theta,$$

the total reflection takes place below certain glancing angle θ_c, a critical angle, given as

$$\sin\theta_c = (eV_0/E_0)^{1/2}.$$

In case of silicon surfaces, since eV_0 is 12 eV [1], the critical angle becomes 2° for 10 keV positrons. This value is quite large in RHEPD experimental arrangement.

At the total reflection condition, the surface normal wave number is imaginary as mention above. Therefore the wave in the crystal becomes evanescent wave. Using the imaginary value of the wave number, it is easily estimated penetration depth of positrons as less than 0.1 nm at the total reflection condition as shown in Fig. 1. Therefore it is able to detect only the topmost layer effects without bulk effects by RHEPD at the total reflection condition [2-5].

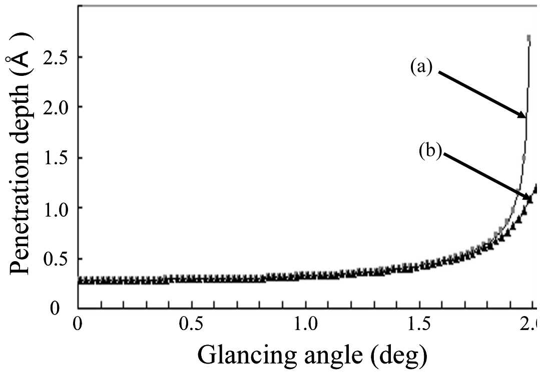

Fig. 1 Glancing angle dependences of penetration depth of evanescent waves for a 10 keV positron beam in a silicon substrate with mean inner potential of 12 V. Curve (a) for no absorption of positron beams and curve (b) for mean imaginary potential (absorption potential) of 1.5 V.

At the total reflection condition, it is necessarily to calculate RHEPD intensities using dynamical diffraction theory for fast positrons. The dynamical theory for RHEPD is the same as the theory for reflection high-energy electron diffraction (RHEED) because the absolute values of the mass and the charge are the same but the sign of the charge is opposite. So we are able to use the RHEED dynamical theory [6] for the RHEPD intensity analysis.

We show some examples of RHEPD dynamical analyses for several surface structure on Si(111) surfaces at the total reflection condition.

References

[1] A. Ichimiya.: *Surf. Sci. Lett.*, **192**, L893-L898 (1987).

[2] A. Ichimiya: Solid State Phenom., **28&29**, 143-147 (1992/93)..

[3]A. Kawasuso, M. Yoshikawa, K. Kojima, S. Okada and A. Ichimiya: Phys. Rev. B**61**, 2102-2106 (2000).

[4] A. Kawasuso *et al.*: Phys. Rev. B **68**, 241313 (2003).

[5]Y. Fukaya, A. Kawasuso and A. Ichimiya, Phys. Rev. B**75** (2007) 115424-115430.

[6] A. Ichimiya: Jpn. J. Appl. Phys. **22**, 176-180 (1983).