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Reflection High-Energy Positron Diffraction: Solved and Unsolved Problems

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Reflection high-energy positron diffraction (RHEPD) as a surface tool has been established. In this report, we show our experimental method with several examples for Si, SiC and metal surfaces. Present problems and feature plan are also argued.

Reflection high-energy positron diffraction (RHEPD) is a surface tool which is realized using positron diffraction phenomenon on crystal surface at small glancing angles (<5°) [1,2]. The experimental setup is equivalent to reflection high-energy electron diffraction (RHEED) except using positrons instead of electrons. Most striking difference of RHEPD from RHEED is the appearance of total reflection [3,4]. Positrons are totally reflected at topmost surface below a critical glancing angle ($\theta<\arcsin(eV_0/E)^{1/2}$) due to positive crystal potential. In the total reflection region, diffraction intensity should be sensitive to surface state, such as atomic irregularity, adsorption, lattice vibration [4]. This is the advantage to use RHEPD in the surface study.

Figure 1 shows a schematic view of our RHEPD experimental setup. The apparatus is composed of the positron gun with 370 MBq ^{22}Na, three Einzel lenses, an electrostatic deflector and a beam collimator. In the fabrication of the positron gun, we followed the Brandeis method which is well established for low energy positron diffraction (LEPD) [5]. Characteristics of Einzel lens is evaluated using the tables given by Harting and Read [6]. Positrons are accelerated by electrical floating of the positron gun and the first Einzel lens as shown in Fig. 1. The beam energy is variable from 10 to 20 keV in this system. We prefer to make RHEPD experiments at 20 keV to have a better beam. Using the long-length collimator (1 mm diameter), non-axial beam was cut off and axial beam was selected. The details of beam development is described elsewhere [4]. The energy spread of this beam is approximately ±200eV.

We obtained RHEPD patterns from various solid surfaces [1,2,7,8]. As an example, Fig. 2 shows the RHEPD patterns for a 6H-SiC(0001) surfaces at different crystallographic orientations. It is seen that these patterns certainly reflect the 1x1 atomic configuration. It was also revealed that the arrangement of observed spots are similar to that obtained in RHEED. This is reasonable since diffraction pattern itself is a projection of surface reciprocal lattice.

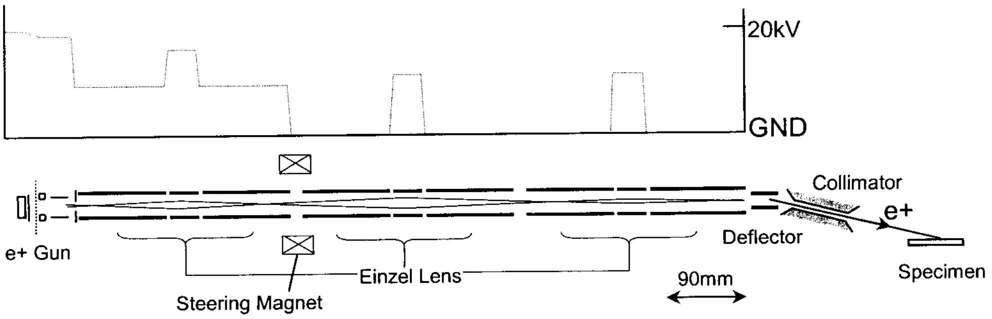

Fig.1 Schematic diagram of RHEPD beam apparatus and electric potential of each component.

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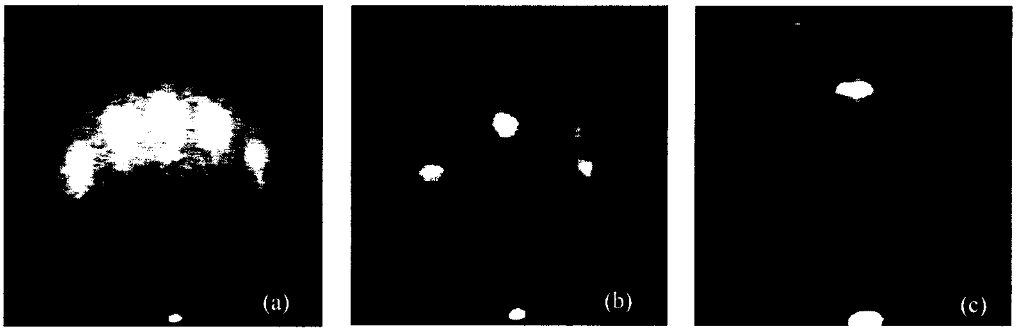

Fig. 2 RHEPD diffraction patterns from 6H SiC(0001) surface at (a) [1120], (b) [1100] incidences, and (c) in one-beam condition (7.5° off from [1100] direction).

As stated above, the effect of total reflection is seen in the rocking curve. The normalized rocking curve for an atomically flat 6H SiC(0001) is shown in Fig. 3 [8]. The experimental data agrees with the dynamical calculation by Ichimiya's method [9]. From the calculation, the total reflection region is below 1.7°. The consistency between theory and experiment suggests that rocking curve exactly provides crystal potential. From Fig. 3, we can also find the first Bragg reflection around 1.9° which do not appear in RHEED experiment.

Change in the surface potential gives a distinct dip structure in the rocking curve in the total reflection region. Actually, such effects were reported for hydrogen-terminated Si(111) and SiC(0001) surfaces [7,8]. Although structure of adsorbed layer can also be determined from RHEPD rocking curve, this has not yet been performed. Determination of surface Debye temperature without any disturbance from bulk is proposed to be possible in RHEPD experiment. To perform this kind of experiment, positron beam itself should be sophisticated more.

Total reflection is also observed in LEPD [10]. In LEPD experiment, however, inelastic scatterings like plasmon excitation and positronium formation, are not negligible and hence *I-V* data analysis would be a complicated matter in some cases. Polarization due to the approach of positrons to surface disturbs the precise determination of crystal potential. On the contrary, in RHEPD experiment, such processes are much reduced [11]. This is recognized from Fig. 3 in which the experimental rocking curve in the total reflection region is well described by a dynamical calculation without such inelastic processes. Thus, RHEPD experiment in total reflection region provide much direct information concerning with surface.

One important application of RHEPD is the determination of metal surface dipole barriers since there is no suitable technique to determine

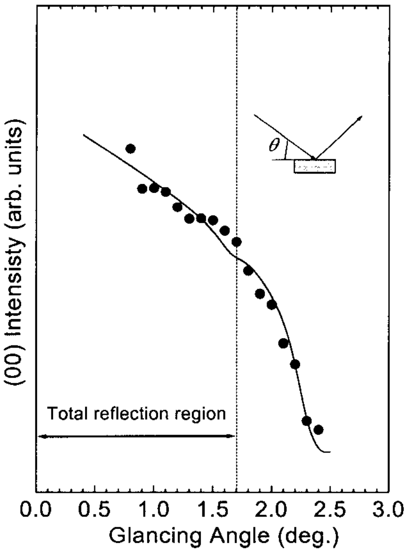

Fig. 3 Specular spot intensity as a function of glancing angle (solid circle) and theoretical rocking curve (solid line) from 6H SiC(0001).

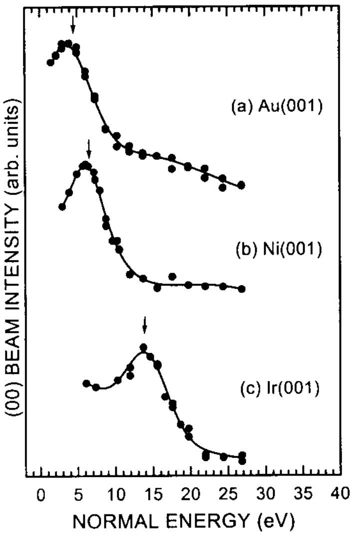

Fig. 4 Specular intenrity for some metals as a function of normal positron energy (=Esin$^2\theta$).

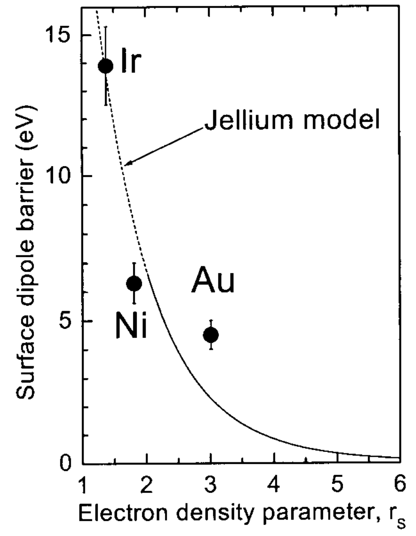

Fig.5 Surface dipole barrier by jellium approximation and threshold energies for three metals shown in Fig.4.

this physical quantity except RHEPD. Figure 4 shows positron reflectivity for Ni, Au and Ir (001) surfaces [4]. According to Oliva [1], threshold energy for the abrupt drop of reflectivity gives the dipole barrier of a metal. Figure 5 shows such threshold energies shown by arrows in Fig. 4 as a function of electron density parameter with surface dipole barrier evaluated from the jellium approximation [12]. The experimental points are comparable to the theoretical prediction. Although this seems to be plausible in light of Oliva's prediction, to confirm if RHEPD gives surface dipole barrier, we need more detailed theoretical calculation and further experimental data with much well defined surfaces.

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