Correlation between Auger Intensity and Wave-Field Intensity for Si(001)2×2-Al Surface*

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According to dynamical theory of electron diffraction, the incident electron density distribution, or “wave-field”, was calculated for a parallel-dimer structure of Si(001)2×2-Al surface on the condition of medium-energy electron diffraction (MEED). The surface structure and the calculated method were confirmed to be effective by the rocking-curve analysis of diffracted beam intensity. The wave-field at the surface is very sensitive to changes in diffraction conditions, such as the incident glancing angle. The Al(LMM) Auger electron intensity emitted from the Si(001)2×2-Al surface during MEED incident beam rocking, that is named beam rocking Auger electron spectroscopy (BRAES), has been found to be correlated to the calculated wave-field intensity on the Al atomic rows. The BRAES profile of adsorbate Al(LMM) differs from that of substrate Si(LVV).

Keywords: Electron diffraction; Auger ejection; Silicon; Aluminum; Superlattices; wave-field; dynamical calculation; Si(001)2×2-Al

I. INTRODUCTION

In current nanotechnology, not only the ability of nano-construction, but also the ability of nano-analysis is important. There are two groups for the analytical methods of surface structure; one consisting of scanning probe methods and the other comprised of diffraction methods. The former is real space observation in local surface area and the latter is reciprocal space observation of averaged surface structure over the beam irradiated area. Here, we are interested in reflection electron diffraction method such as medium-energy electron diffraction (MEED) or reflection high-energy electron diffraction (RHEED). The reflection electron diffraction method is powerful tool for surface structure analysis, however, it is generally difficult for this method to distinguish which elements form a surface, especially elements with similar atomic numbers.

Our final purpose is to develop the analysis method of adatom site for adsorbed surface system by the combination of reflection electron diffraction and Auger electron spectroscopy (AES). Auger electrons excited by the incident electron beam of MEED or RHEED have information on the surface structure. Emission process of Auger electrons from the point sources, such as Auger electron diffraction or focusing effect, was inclusively reviewed by Chambers [1]. Focusing and defocusing effects of the emitted Auger electrons were also examined by Valeri et al. [2]. Many researches described in the above review paper [1] were mainly carried out by use of angle-resolved detector which was scanned in wide angle range passing through certain low-index directions of sample crystal. Auger intensity increases at such low-index directions due to the focusing effect.

On the other hand, we used LEED optics as a retarding field analyzer. The diffraction effect of emitted Auger electrons is ignored because the used detector is a spatially integrated type analyzer. We do not pay attention to the emission process of Auger electrons, but to the excitation process of them. For crystal surface, the incident electron beam forms a periodic electron density distribution, or “wave-field”, in the vicinity of the surface due to interference between diffracted electron beams [3, 4]. When the intensity of the wave-field is strong on certain atomic rows, the Auger intensity from these atoms is expected to be enhanced. This assumption may be applied to a new surface structure analysis technique to allow identification of elements. We previously measured Auger electron intensity while changing the glancing angle of the incident electron beam. The glancing angle dependence of Auger intensity is called a “beam rocking Auger electron spectroscopy (BRAES)” profile. Intensity anomalies on the BRAES profiles have been found for several surface structures [5–8].

The wave-field changes depending on the glancing angle of the incident electron beam. If the wave-field intensity increases on certain atomic rows, it is expected that the Auger electron intensity from these atomic rows would be enhanced. In order to confirm this assumption for Si(001)2×2-Al surface, we examined the correlation between the wave-field and Auger electron intensity while changing the incident angle. If the correlation is confirmed, the new structure analysis method becomes a realistic possibility, and may be considered a complementary method to the usual reflection electron diffraction. The characteristic point of this study is that we use the Auger electron intensity not only to identify an element, but also in analysis of the adsorption site.

II. EXPERIMENTAL

The experiment was done using an ultra-high vacuum RHEED apparatus equipped with LEED optics (OCI Vacuum Microengineering) as shown in Fig. 1. The glancing angle of the incident electron beam was controlled mechanically from 0° to 6° with an angular resolution of 0.01°. The usual incident electron energy for RHEED is 10 keV or higher, however a 5 keV incident electron beam

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was used in this study, which corresponds to MEED conditions. Because it is considered that the medium-energy electron beam generally gives a higher Auger electron excitation than high-energy electron beam.

The entrance plane of LEED optics, a retarding field analyzer, is placed about 15 mm above the sample surface, and used to detect Auger electrons. It is possible to move the analyzer 50 mm above the sample surface at the deposition of Al. A built-in electron gun is not supplied with this LEED optics, because the LEED optics is merely used as a retarding field analyzer. A Kikuchi pattern can be observed on the LEED optics during MEED, as described in ref. [9], where the hemispherical LEED screen is called an “astrodome screen”. As the LEED optics were used as a spatially integrated type analyzer for the detection of Auger electrons, Auger diffraction effects may be neglected.

The used sample is a Si(001)2£2-Al surface, which is formed by 1/2 monolayer deposition of Al onto a clean double-domain Si(001)2£1 surface at room temperature. The incident azimuth was set in the [100] direction, which forms an angle of 45° with each of the two orthogonally-arrayed Si dimer rows in each domain. Use of this azimuth removes the complicated influence of the double domains in the calculations of diffracted beam intensities.

Experimental rocking-curves of diffraction spot intensities were captured from the MEED pattern image data by a CCD camera while the incident electron beam angle was changed in 0.1° increments. Auger electron intensities were measured while continuously varying the glancing angle. The measured Auger peaks are Al(LMM) with a kinetic energy of 68 eV and Si(LVV) with that of 92 eV.

III. RESULTS AND DISCUSSION

Rocking-curves of 0 0, 1/2 1/2 and 1 1 diffraction spots have been measured at [100] azimuth with 5 keV incident beam and these experimental results are shown in Fig. 2 by solid lines.

For Si(001)2£2-Al surface structure, parallel-dimer and orthogonal-dimer structural models have been proposed. The parallel-dimer model, in which Al dimers and Si dimers are parallel to each other as shown in Fig. 3, is believed to be more reliable because of its significantly lower surface energy [10]. We therefore analyzed the experimental rocking-curve using the parallel-dimer model with structural parameters proposed by Sakama et al. [11]. The dynamical calculation has been carried out by using a multi-slice method [12, 13], in which the sample was sliced at 0.1 Å intervals down to about 100 Å in depth. Fourier coefficients of the two dimensional crystal potential were calculated using the parameters of Doyle and Turner [14], then the Schrödinger equation was solved within each slice. Debye-Waller factors due to the atomic vibrations of Al and Si were taken into account by using Radi’s data [15], where the Debye temperatures of Si and

http://www.sssj.org/ejssnt (J-Stage: http://www.jstage.jst.go.jp/browse/ejssnt/)
Al are 580 K and 390 K at room temperature (20°C), respectively. The nine beams given by 0 0, ±1/2 ± 1/2, ±1 ± 1, ±3/2 ± 3/2, and ±2 ± 2 (the same double-sign order) were taken into account in the rocking-curve calculations.

The calculated results of the rocking-curves are shown in Fig. 2 by the broken lines, where it can be seen that the experimental rocking-curves are reproduced relatively well by the calculations. As a diffraction spot intensity at the beginning of the emergence generally suffers the absorption by strong surface plasmon losses and the refraction at surface step edges, the experimental intensity tends to decrease compared with the calculated one as seen in 1 1 and 0 0 spots in Fig. 2. This may be the reason why the peak intensity of 1 1 spot is weak at \( \theta = 4^\circ \) near the emergence angle 3.6° and the intensity of 0 0 spot at \( \theta \lesssim 1.5^\circ \). For the rocking curve of 1/2 1/2 half-order spot, however, the experimental intensity arises before the emergence angle, \( \theta = 1.8^\circ \). This is due to the especially streaky shape of the half-order spot, which appears weakly even before the emergence. For the parallel-dimer model, relatively good agreement between the experimental and the calculated rocking curves has been also confirmed in the RHEED condition with 10 keV incident beam, where the more peaks of higher-order in the rocking curves were compared to each other. Therefore the parallel-dimer model is confirmed to be reliable for the Si(001)2×2-Al surface structure.

The wave-field formed in the vicinity of the crystal surface has been calculated for this parallel-dimer model, and the results are shown in Fig. 4. The computation region is the interior of the rectangular frame shown in Fig. 3(b). The transverse length is 7 Å and longitudinal length is 9 Å on the frame which is perpendicular to the incident
In [100] incident azimuth, Si atomic rows in ideal (bulk calculated wave-fields for the glancing angles from substrate Si atomic rows, respectively. Fig. 4 shows the “azimuth [100] of the electron beam. Here, the symbols closed and open circles, respectively. lated wave-field intensity on Al atomic rows are indicated by sphere is denoted by its glancing angle. Open circles indicate into account of mean inner potential of Si, 12 eV. Each Ewald sphere is taken by the 0-th Laue zone. Radius of the Ewald sphere is taken of mean inner potential of Si, 12 eV. Each Ewald by the 0-th Laue zone. Radius of the Ewald sphere is taken into account of mean inner potential of Si, 12 eV. Each Ewald satisfaction as shown in Fig. 5 and a standing wave with an interval of a/4 appears perpendicular to the surface. Phase of the standing wave gradually move to inside transforming its shape as the glancing angle increases. The side beams, 1 1 and 1 1, begin to appear inside the crystal at θ=2.4° as seen in Fig. 5, however these beams cannot escape the surface until θ=3.5° by refraction effect. These side beams propagate parallel to the surface and form a very strong wave-field underneath the surface. The diffraction condition in this glancing-angle range corresponds to a so-called “surface wave resonance (SWR)” condition. At θ=2.7° or 2.8°, intensities of the half order beams become minimum and the vacuum wave-field is mostly formed by simple interference of incident beam and specular beam. Therefore the wave-field in vacuum shows uniform standing wave.

Above θ=3.5°, side beams of 1 1 and 1 1 begin to emerge from the surface. At θ=4.0°, these side beams meet a peak intensity and modulate the wave-field in vacuum with a periodicity of a/2 parallel to the surface.

Behavior of the wave-field depending on the incident azimuth angle is very interesting. At low glancing angle of θ=2.1°, incident beam does not enter the crystal so much and most of the beam is reflected into vacuum. Wave-field in vacuum shows the periodic modulation of lattice constant a=5.43 Å in the surface parallel direction. In [100] incident azimuth, Si atomic rows in ideal (bulk terminated) surface arrange at intervals of a/2, however, 2×2 periodicity of super structure produces modulation with twice larger period, a, in vacuum wave-field. Actually, intensities of 1/2 1/2 and 1/2 1/2 half order beams meet a peak around θ=2.0° as seen in Fig. 2.

At θ=2.4°, the Bragg condition of 0 0 4 reflection is satisfied as shown in Fig. 5 and a standing wave with an interval of a/4 appears perpendicular to the surface. Phase of the standing wave gradually move to inside transforming its shape as the glancing angle increases. The side beams, 1 1 and 1 1, begin to appear inside the crystal at θ=2.4° as seen in Fig. 5, however these beams cannot escape the surface until θ=3.5° by refraction effect. These side beams propagate parallel to the surface and form a very strong wave-field underneath the surface. The diffraction condition in this glancing-angle range corresponds to a so-called “surface wave resonance (SWR)” condition. At θ=2.7° or 2.8°, intensities of the half order beams become minimum and the vacuum wave-field is mostly formed by simple interference of incident beam and specular beam. Therefore the wave-field in vacuum shows uniform standing wave. Above θ=3.5°, side beams of 1 1 and 1 1 begin to emerge from the surface. At θ=4.0°, these side beams meet a peak intensity and modulate the wave-field in vacuum with a periodicity of a/2 parallel to the surface.

The wave-field exhibits a sensitive dependence on the glancing angle. It is seen in Fig. 4 that the incident electrons generally localize at the inter-atomic rows rather than the atomic rows. This phenomenon may correspond to an electron channeling phenomenon along inter-atomic rows, which is also recognized in the wave-field of RHEED with 10 keV incident beam.[16]

It can be seen in Fig. 4 that the wave-field intensity on Al atomic rows, whose locations are indicated by “×” and “+” denote the positions of adsorbed Al and substrate Si atomic rows, respectively. Fig. 4 shows the calculated wave-fields for the glancing angles from θ=2.1° to 4.5° at 0.1° intervals. All wave-field intensities are represented by the fixed gray scale with a maximum value of 3.5. When the wave-field intensity exceeds this maximum value, the region is colored black, as seen in 2.7°, 2.9° and 3.1°.

Behavior of the wave-field depending on the incident glancing angle is very interesting. At low glancing angle of θ=2.1°, incident beam does not enter the crystal so much and most of the beam is reflected into vacuum. Wave-field in vacuum shows the periodic modulation of lattice constant a=5.43 Å in the surface parallel direction. In [100] incident azimuth, Si atomic rows in ideal (bulk described). FIG. 5: Cross section of Ewald sphere in Si crystal cutted by the 0-th Laue zone. Radius of the Ewald sphere is taken into account of mean inner potential of Si, 12 eV. Each Ewald sphere is denoted by its glancing angle. Open circles indicate into account of mean inner potential of Si, 12 eV.

FIG. 6: Experimental BRAES profile of Al(LMM) and calculated wave-field intensity on Al atomic rows are indicated by closed and open circles, respectively.

Azimuth [100] of the electron beam. Here, the symbols “×” and “+” denote the positions of adsorbed Al and substrate Si atomic rows, respectively. Fig. 4 shows the calculated wave-fields for the glancing angles from θ=2.1° to 4.5° at 0.1° intervals. All wave-field intensities are represented by the fixed gray scale with a maximum value of 3.5. When the wave-field intensity exceeds this maximum value, the region is colored black, as seen in 2.7°, 2.9° and 3.1°.

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ent locations of Si and Al atomic rows. Si(LVV) BRAES profiles taken from Si(001)2×2-Al surface and from clean Si(001)2×1 surface are similar to each other especially in the main peak position of 3.2°, but small disagreements are seen at 2.4°, 2.6°, 4.2°, and 4.8°. These disagreements are considered to be due to the relaxation of the substrate Si structure induced by Al adsorption, however, the Si-dimer structure of the clean Si(001)2x1 surface is preserved in 2×2-Al surface.

IV. CONCLUSION

The surface structure of Si(001)2×2-Al was confirmed to match a parallel-dimer model by rocking-curve analysis of diffraction intensities. Wave-fields formed within the surface were calculated using dynamical theory and employing the parallel-dimer model. The calculated wave-field changes sensitively depending on the glancing angle of the incident beam. It has been found that the behavior of Auger electron intensity of Al(LMM) emitted from a Si(001)2×2-Al surface is similar to that of the calculated wave-field intensity on Al atomic rows. On the other hand, BRAES profile of Si(LVV), which comes from substrate Si, is different from that of Al(LMM). The behavior of the wave-field is not only of academic interest, but may be also applicable to the analysis of adsorbed surface structures as a complementary method to MEED or RHEED.

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