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Evaluation of the Roughness of a Crystal Surface by X-ray Scattering. I. Theoretical Considerations

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Abstract

The relationship between the intensity distributions of the crystal truncation rod (CTR) scattering and the surface roughness of a crystal is discussed by developing a kinematic theory for the CTR scattering so as to reflect the two-dimensional aspect of the surface. The intensity of the CTR scattering elongated from a Bragg point is shown to be reduced by a factor $|\Gamma(q)|^2$ for a surface possessing some roughness, where $\Gamma(q)$ is defined by a simple Fourier summation of γ_p, the relative area with the same step height p on a surface, *i.e.* $\Gamma(q)=\sum_{p=0}^{\infty}\gamma_p \exp(2\pi ipq)$, with $\sum_p \gamma_p = 1$, q being the distance in reciprocal space from the Bragg point along the CTR scattering. A pair-correlation function between the steps can, therefore, be obtained by a simple Fourier integral of the roughness damping factor $|\Gamma(q)|^2$. For the case where γ_p has a Gaussian distribution around the average step height, $|\Gamma(q)|^2$ is approximated by the well known Debye-Waller-like factor, $\exp(-4\pi^2\langle\Delta p^2\rangle q^2)$, where $\langle\Delta p^2\rangle$ is the mean square deviation of step height in units of the lattice spacing. The intensity formulae proposed so far by several authors are also discussed on the basis of the above factor.

Introduction

The effect on the diffraction pattern of the abrupt truncation of a crystal at the surface is to give rise to rod-shaped scattering elongated from each Bragg point in a direction normal to the crystal surface. The rod-shaped scattering is referred to as crystal truncation rod (CTR) scattering in X-ray diffraction. The intensity distribution along the rod depends very much on the condition of the surface, such as the surface roughness and the surface lattice relaxation. Thus, the analysis of the CTR scattering can provide valuable information on the lattice modulation at a crystal surface and also on the interface boundary on an atomic scale, as demonstrated by several authors. Andrews & Cowley (1985) showed that the intensity of the CTR scattering is proportional to the inverse square of the distance from the Bragg point for the ideally flat surface but falls off from it by a Debye-Waller-like factor for a surface with some roughness. On the other hand, Robinson (1986) showed that surface morphology of an Si(111) surface can be discussed on an atomic scale on the basis of the CTR scattering. Afanas'ev, Aleksandrov, Fanchenko, Chaplanov & Yakimov (1986) and Kashihara, Kawamura, Kashiwagura & Harada (1987) pointed out that it is also possible to evaluate the surface lattice relaxation if, in addition, the asymmetry of the CTR scattering with respect to the Bragg point is taken into account.

In representing the intensity modulation along the CTR scattering due to surface roughness, other theoretical approaches have also been proposed by Vlieg, van der Veen, Gurman, Norris & Macdonald (1989) and Kashihara (1990). However, the extent of the validity for the formulae presented and also their relationships have not so far been clarified. It is, therefore, important to assess the validity of these formulae in order to evaluate the roughness of various

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crystal surfaces from the analysis of the X-ray CTR scattering and this is one of the aims of the present study. Here, in paper I of the study, we discuss firstly the effect of surface roughness on the intensity along the CTR scattering on the basis of a kinematical theory of diffraction. In paper II we present an efficient new technique, using imaging plates, to estimate the surface roughness of any crystal from the analysis of the X-ray CTR scattering on the basis of the formula presented in this paper.

Formulation of CTR scattering

For simplicity we will consider a semi-infinite crystal of orthogonal lattice with lattice parameters a, b and c along the orthogonal x, y and z axes, respectively. Only one atom is assumed to be in the unit cell. Fig. 1(a) shows a section of such a lattice with the extended surface, in which some irregularity exists due to steps and holes on the surface. In general, a lattice relaxation may also exist, accompanying the abrupt change in atomic density at the surface. However, at the beginning we consider the case where no lattice relaxation occurs on the surface. The vector representing a lattice site is labeled by three integers m, n, p:

$$\mathbf{r}_{mnp} = m\mathbf{a} + n\mathbf{b} + p\mathbf{c}, \tag{1}$$

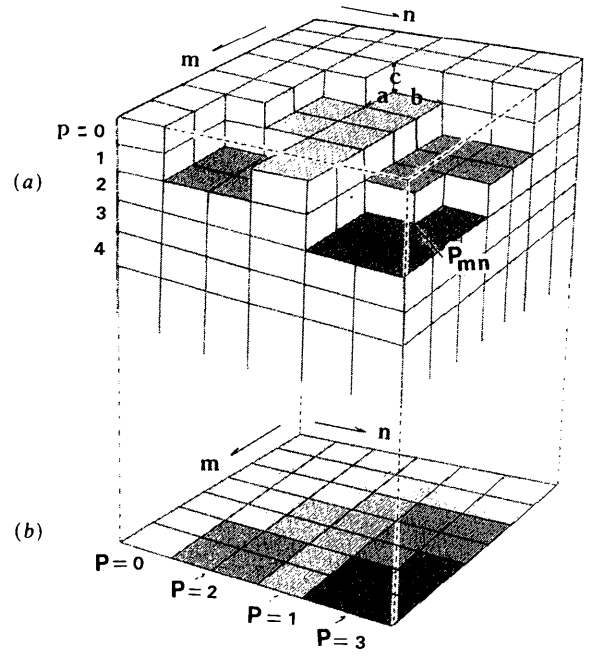


Fig. 1. (a) A part of an orthogonal lattice, the surface of which has several kinds of steps, where a, b and c are the lattice parameters and p_{mn} is the step height at the (m, n)th lattice point. (b) Two-dimensional lattice with phase modulation (shaded), reduced from the three-dimensional lattice with steps on the surface of (a).

where m and n take values from $-\infty$ to $+\infty$ but p takes values from $-\infty$ to 0. The scattering amplitude from this crystal lattice is given by simply summing up all the phase factors as

$$F(K_x, K_y, K_z) = \sum_m \sum_n \sum_p f(K) \exp[i(K_x ma + K_y nb + K_z pc)], \tag{2}$$

where K_x, K_y and K_z are the components of the scattering vector $\mathbf{K}$ relative to the orthogonal axes x, y, z [$|\mathbf{K}| = 4\pi(\sin\theta)/\lambda$, 2θ being the scattering angle and λ the wavelength] and $f(K)$ is the atomic scattering factor. It will be abbreviated as f according to circumstances.

In the derivation of a general formula for the intensity distribution of CTR scattering, it is convenient to sum first phase factors along the direction normal to the surface and then to take the summation over the lateral directions. That is, the summation of (2) is made with respect to p first by keeping m and n constant. We will refer to such a summation as a 'column summation'. The scattering amplitude for the (m, n) column along the z axis is given by

$$\Phi_{mn} = \sum_{p \le p_{mn}}^{-\infty} f(K) \exp(iK_z pc) = \Phi_0 \exp(-iK_z p_{mn} c), \tag{3}$$

with

$$\Phi_0 = f(K)/[1 - \exp(iK_z c)], \tag{4}$$

where p_{mn} is an integer representing the step height from the top lattice point of the (m, n) column to the $p = 0$ level as shown in Fig. 1(a). The scattering amplitude, Φ_{mn}, for the (m, n) column is, therefore, expressed as the product of the 'column form factor', Φ_0, and the 'column phase factor', $\exp(-iK_z p_{mn} c)$.

With the use of Φ_{mn} the scattering amplitude from all the lattice points can be reduced to a two-dimensional lattice sum,

$$F(K_x, K_y, K_z) = \sum_m \sum_n \Phi_{mn} \exp[i(K_x ma + K_y nb)]. \tag{5}$$

The intensity is proportional to the square of the scattering amplitude, so that we have

$$I(K_x, K_y, K_z) = F(K_x, K_y, K_z) F^*(K_x, K_y, K_z) = \sum_m \sum_n N_{mn} \langle \Phi \Phi^*_{mn} \rangle \exp[i(K_x ma + K_y nb)], \tag{6}$$

where the symbol $\langle \Phi \Phi^*_{mn} \rangle$ indicates the average of all the pair correlations between the two columns that are separated by $\mathbf{r}_{mn} (= \mathbf{r}_{m+m', n+n'} - \mathbf{r}_{m'n'})$ over the whole crystal and N_{mn} is the number of such possible pairs of columns. It should be noted that (6) is in the form of the scattering from a two-dimensional lattice

if we regard Φ_{mn} as a pseudo form factor located at the (m, n) lattice point. It may also be interpreted as a two-dimensional lattice with the phase modulation related to the step height as shown in Fig. 1(*b*). Thus, it is possible to treat (6) as the scattering from a two-dimensional lattice.

Now, following Cowley (1981), we can introduce the average column form factor, $\langle\Phi_{mn}\rangle$, defined as

$$\Phi_{mn} = \langle\Phi_{mn}\rangle + \Delta\Phi_{mn}, . \tag{7}$$

where $\Delta\Phi_{mn}$ is the deviation from the average column form factor $\langle\Phi_{mn}\rangle$ at the (m, n) lattice point. If $\langle X\rangle$ indicates the average of X for all the lattice points, we have $\langle\Phi_{mn}\rangle = \langle\Phi\rangle$. With use of (7), the pair correlation $\langle\Phi\Phi^*_{mn}\rangle$ in (6) is given by

$$\langle\Phi\Phi^*_{mn}\rangle = \langle\Phi\rangle^2 + \langle\Delta\Phi\Delta\Phi^*_{mn}\rangle. \tag{8}$$

By substituting (8) into (6), we have

$$\begin{aligned} I(K_x, K_y, K_z) &= \langle\Phi\rangle^2 \sum_m \sum_n N_{mn} \exp[i(K_x ma + K_y nb)] \\ &+ \sum_m \sum_n N_{mn} \langle\Delta\Phi\Delta\Phi^*_{mn}\rangle \\ &\times \exp[i(K_x ma + K_y nb)]. \end{aligned} \tag{9}$$

The first term on the right-hand side is the Bragg scattering from a crystal with the average surface. The second term is the diffuse scattering, which arises from the existence of the irregularity or roughness of the surface. If the surface is ideally flat, this term disappears.

CTR scattering

In this section, we discuss the factor $\langle\Phi\rangle$ in the Bragg term of (9) especially the effect of the irregularity of the surface on the Bragg term. From (3), for Φ_{mn} we have

$$\langle\Phi\rangle = \langle\Phi_{mn}\rangle = \Phi_0\langle\exp(-iK_z p_{mn} c)\rangle. \tag{10}$$

Thus we see that evaluation of the average column form factor is equivalent to taking the average of the column phase factor. Since p_{mn} indicates the step-height deviation from the top surface at column (m, n), we also see that information about surface roughness is included in this average. The scattering vector K_z is written in the form

$$K_z = lc^* + qc^*, \tag{11}$$

where l is the Miller index, representing the reciprocal-lattice point along the K_z direction, q the deviation from it and c^* the reciprocal-lattice unit with the relation $(cc^* = 2\pi)$. The column phase factor is rewritten as

$$\begin{aligned} &\exp(-iK_z p_{mn} c) \\ &\quad = \exp(-2\pi i p_{mn} l) \exp(-2\pi i p_{mn} q). \end{aligned} \tag{12}$$

The first exponential factor of (12) will be unity since p_{mn} and l are both integers. Thus, the average of the phase factor is given as

$$\langle\exp(-2\pi i p_{mn} q)\rangle \equiv \Gamma(q). \tag{13}$$

$\Gamma(q)$ represents the damping factor for the column form factor Φ_0, along the direction K_z normal to the surface, due to surface roughness. Thus, the intensity distribution of the Bragg term is given by

$$\begin{aligned} &I_{\mathrm{CTR}}(K_x, K_y, K_z) \\ &\quad = \Phi_0^2 \Gamma(q)^2 [\sin(K_x Ma/2)/\sin(K_x a/2)]^2 \\ &\qquad \times [\sin(K_y Nb/2)/\sin(K_y b/2)]^2, \end{aligned} \tag{14}$$

where M and N are the total effective number of lattice points in the x and y directions, respectively.

For the case of the perfect flat surface, the surface has no irregularity. Thus all the values of p_{mn} should be zero, so that we have $\Gamma(q) = 1$. Therefore the Bragg scattering has a long tail along the K_z direction, since it varies as $|f(K)/[1-\exp(iK_z c)]|^2$, but is very sharp for the direction perpendicular to it because of the Laue functions along the K_x and K_y directions. The intensity distribution in reciprocal space shows, therefore, a similar aspect to the scattering from a two-dimensional lattice and/or that from a disc-shaped crystal, except for the intensity modulation along the K_z direction, as shown schematically in Fig. 2. The $h, k, l+q$ point is not equivalent to the $l+q, k, h$ point in the reciprocal space, even for cubic crystals. This arises from the requirement that only two-dimensional symmetry around the axis perpendicular

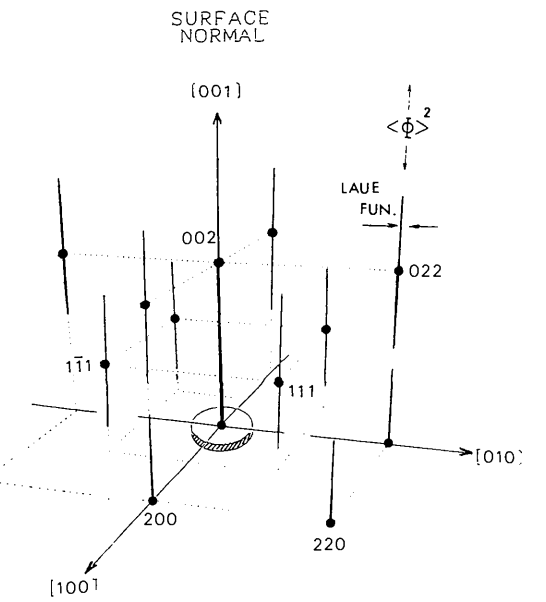


Fig. 2. Intensity distribution in the reciprocal space for a crystal with an extended surface, showing the two-dimensional aspect. The $h, k, l+q$ point is not equivalent to the $h+q, k, l$ point, even for the lattice with cubic symmetry.

to the surface can hold for a crystal with an extended surface, since the surface has to be kept unchanged for such a symmetry operation, as discussed by Kashihara, Kawamura & Harada (1991). It should be noted that this effect is only observed in the scattering from the surface and not in the Bragg scattering. The long tail of Bragg scattering along the K_z direction is in fact the crystal truncation rod (CTR) scattering, although it looks more like a 'needle' than a 'rod'. The effect of the roughness of the surface is seen along the K_z direction in that Φ_0^2 is reduced by the factor $\Gamma(q)^2$, as will be discussed later.

If we can assume that there is no correlation between any pair of columns, *i.e.* the surface is random, the second term of (9), representing the diffuse scattering is reduced to the simple form

$$I_{\mathrm{DIFF}}(K_x, K_y, K_z) = Nf(K)^2[1-|\Gamma(q)|^2]. \quad (15)$$

The diffuse scattering increases monotonously with increasing q along the direction perpendicular to the surface, since $|\Gamma(q)|=1$ at $q=0$ and it approaches the limiting value at $q_{\max}$. On the other hand, it decreases along the direction parallel to the surface because of the factor f^2. As seen from (15), there is a close resemblance between this scattering and the thermal diffuse scattering for a two-dimensional lattice in the Einstein approximation.

Lattice relaxation

We have so far ignored the effect of lattice relaxation at the surface on the CTR scattering. This effect is considerable, giving rise to asymmetry in the CTR intensity as pointed out by Afanas'ev *et al.* (1986) and Kashihara *et al.* (1987). If the lattice relaxation is assumed to decay with depth p from the surface according to the relation $U_p = U_0 \exp(-p/\xi')$, where U_p is the displacement of the lattice spacing at the pth level and ξ' the characteristic depth of the relaxed surface, we may include the effect of lattice relaxation by replacing Φ_0 of (14) with

$$\begin{aligned}\Phi_0' = \Phi_0\{&1+i(K_zU_0)[1-\exp(iK_zc)]\\ &\times[1-\exp(iK_zc-1/\xi')]^{-1}\\ &-(K_zU_0)^2[1-\exp(iK_zc)]\\ &\times[1-\exp(iK_zc-2/\xi')]^{-1}\}\end{aligned} \quad (16)$$

within the approximation $\exp(iKU)\simeq 1+iKU$.

In this treatment the surface lattice relaxation is assumed to be normal to the surface and independent of the lateral direction. It means that no correlation is assumed to exist among the columns with respect to the lattice relaxation. The effect, therefore, should arise only in the Bragg term and not in the diffuse scattering term in (9).

If Φ_0 in (14) is replaced by Φ_0' from (16), we have

$$\begin{aligned}\Phi_0'^2 = &f^2/[2(1-\cos K_zc)]+K_zU\\ &\times 2(\sin K_zc)[1-\exp(-1/\xi')]f^2\\ &\times\{(1-\cos K_zc)\\ &\times[1+\exp(-1/\xi')+\exp(-2/\xi')]\\ &-(\cos K_zc-\cos 2K_zc)\}^{-1}\\ &+\text{term in } (K_zU)^2.\end{aligned} \quad (17)$$

The first term represents the CTR scattering from an ideally flat surface of the crystal. The second and third terms are proportional to the products (KU) and $(KU)^2$, respectively. This is a familiar modulation effect often seen in the X-ray scattering from alloys consisting of atoms with different atomic sizes, when local atomic order exists. They correspond to the size-effect modulation and the well known Huang scattering, respectively, in the short-range-order diffuse scattering from alloys. The second term modulates the intensity of the CTR scattering so as to be asymmetric with respect to the Bragg point, because of the odd function sin K_zc. The third term is negligible compared with the second term and may be ignored.

The effect of the second term can be quite significant in the case of the CTR scattering. Thus it is easy to demonstrate its effect by the use of a simple model. If, for instance, only the top surface layer of a lattice is subjected to the lattice relaxation, the case discussed by Harada, Takata, Miyatake and Koyama (1989) with the use of the optical Fourier transform and also by Vlieg *et al.* (1989), (17) reduces to the simple form

$$\Phi_0'^2 = \Phi_0^2[1+2(K_zU_0)\sin K_zc] \quad (18)$$

as $\exp(-1/\xi')$ tends to zero. On the basis of this relation we easily see that the 1% expansion of the spacing U_0 increases the second term by more than 15% relative to the first term at around $q=0.2$. This is a considerable modulation of the CTR scattering. We also see the sense of lattice relaxation, namely whether lattice expansion or shrinkage occurs, from the intensity asymmetry of the CTR scattering.

Surface roughness

(i) *Roughness damping factor*

We introduce γ_p as the probability of finding columns with a step height p on a crystal surface.

$$\sum_{p\geq 0}\gamma_p = 1. \quad (19)$$

The summations are over all the steps. We see that

$\Gamma(q)$ of (13) is simply given by Fourier summation of this γ_p,

$$\Gamma(q)=\sum_{p=0}^{\infty}\gamma_p\exp\{-2\pi ipq\}. \qquad (20)$$

Thus, the damping factor $|\Gamma(q)|^2$ to the CTR scattering is evaluated by (20) if γ_p is given. $|\Gamma(q)|^2$ will be referred to as the roughness damping factor, RDF, hereafter.

A simple example is the case where only a single kind of step exists on a flat surface as shown in Fig. 3, which is often referred to as a two-level model. $\Gamma(q)$ is expressed by two Fourier components with one parameter γ_0, since γ_1 is equal to $(1-\gamma_0)$ from (19). It should be noted that γ_0 represents the coverage of the top layer on the surface whatever lateral correlation exists between the columns or steps. We have

$$|\Gamma(q)|^2=1-2\gamma_0(1-\gamma_0)(1-\cos 2\pi q). \qquad (21)$$

This result shows that the RDF $|\Gamma(q)|^2$ is a function falling off from 1 at $q=0$ to $1-4\gamma_0(1-\gamma_0)$ at $q=\frac{1}{2}$ for the Brillouin-zone boundary and also an upward parabolic function with respect to the coverage γ_0. If the coverage γ_0 increases with constant speed as seen in the surface grown layer by layer, $|\Gamma(q)|^2$ is expressed in a quadratic form with respect to the time, as shown in Fig. 4. This is a well known relation for the LEED and RHEED oscillations (Neave, Joyce, Dobson & Norton, 1983; Lent & Cohen, 1984) although the oscillation is subject to the effect of dynamical diffraction in the case of electron scattering, but it may hold for X-ray CTR scattering. Vlieg, van der Gon, van der Veen, Macdonald & Norris (1988), however, found that the experimentally observed curve deviates from this simple relation, indicating that the two-level model is not sufficient for a crystal growth of Ge on an Si surface. For (21) such a quadratic relation holds not only for $q=\frac{1}{2}$ at the Brillouin-zone boundary but also for any q value.

For the small q region, such as the points near the Bragg point, $|\Gamma(q)|^2$ is expressed in the form of a Debye–Waller-like factor, $\exp\{-4\pi^2[\gamma_0(1-\gamma_0)]q^2\}$, so that in principle it is possible to estimate the coverage γ_0 even from the analysis of the CTR scattering observed near the Bragg point.

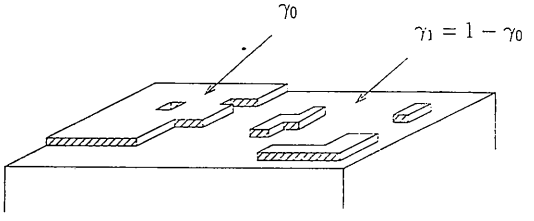


Fig. 3. An illustration of a crystal surface for the two-level model. It is characterized by one parameter γ_0, representing the coverage of the surface.

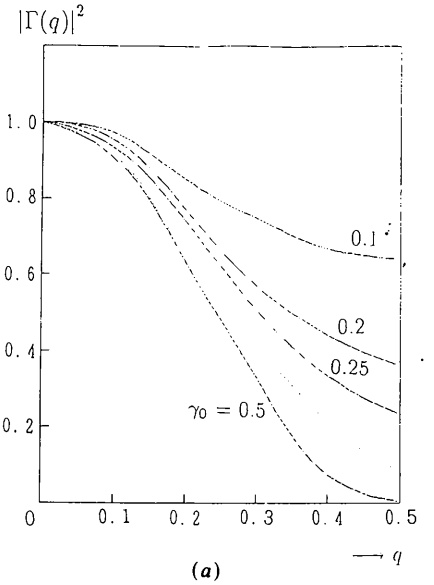
In (20) we see that a pair-correlation function between the steps can be obtained by a simple Fourier integral of the RDF, $|\Gamma(q)|^2$,

$$\langle\gamma_0\gamma_p\rangle=2\int_0^{q_{\max}}|\Gamma(q)|^2\exp(2\pi ipq)\,dq, \qquad (22)$$

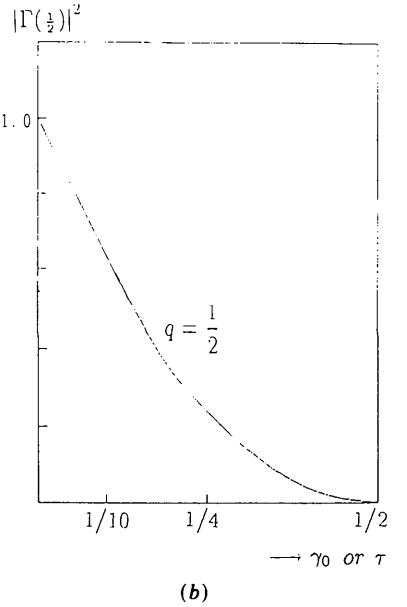
where $\langle\gamma_0\gamma_p\rangle$ is the pair-correlation function defined as

$$\langle\gamma_0\gamma_p\rangle=\sum_{p'>0}\gamma_{p'}\gamma_{p'+p}. \qquad (23)$$

More direct information about γ_p can also be



(*a*)



(*b*)

Fig. 4. The RDF, *versus* (*a*) q and (*b*) γ_0, for the two-level model. The dotted curve shows a Gaussian approximation for $\gamma_0=0.5$.

obtained if $\Gamma(q)$ is known from experiment,

$$\gamma_p = 2 \int_0^{q_{max}} \Gamma(q) \exp(2\pi i p q)\, dq. \quad (24)$$

This result expresses the probability of finding columns with step height p in terms of the Fourier integral of $\Gamma(q)$ as a function of q. Although one may expect to encounter some experimental difficulties in obtaining $\Gamma(q)$ and $|\Gamma(q)|^2$ for the real crystals from the analysis of the CTR scattering, this is a very interesting subject to explore by experiment.

(ii) *Debye-Waller-like factor*

If an average step height $\langle p \rangle$ is introduced, the step height p_{mn} at column (m, n) is given by the sum of $\langle p \rangle$ and the deviation Δp_{mn} from it,

$$p_{mn} = \langle p \rangle + \Delta p_{mn}. \quad (25)$$

The average $\langle p \rangle$ should be taken over the whole two-dimensional pseudolattice. Thus, as illustrated in Fig. 5, $\langle p \rangle$ and its deviation Δp_{mn} are no longer integers and, furthermore, Δp_{mn} can be positive or negative depending on the lattice point (m, n). If we substitute (25) into (13) and take its average, we have

$$\Gamma(q) = \langle \exp(-2\pi i \Delta p_{mn} q) \rangle, \quad (26)$$

where a simple phase factor $\exp(-2\pi i \langle p \rangle q)$ is omitted, as it does not come into the intensity expression. Only the second term of (25) is significant. In the small-q region, it is possible to use the well known relation for taking the average,

$$\langle \exp(-i\alpha) \rangle = \exp(-\tfrac{1}{2}\langle \alpha^2 \rangle), \quad (27)$$

which is exact when α is normally distributed about $\alpha = 0$. We have a similar expression to the Debye-Waller factor for thermal vibration for $\Gamma(q)$,

$$\Gamma(q)^2 = \exp\{-4\pi^2 \langle \Delta p_{mn}^2 \rangle q^2\}, \quad (28)$$

where $\langle \Delta p_{mn}^2 \rangle$ is written as $\langle \Delta p^2 \rangle$. It should be noted that this exponential factor works as a damping factor for the CTR scattering due to surface roughness. This is the same formula as that derived by Andrews & Cowley (1985) by assuming the surface roughness is given by a Gaussian form. The representation (28) is only valid for small q or for the case where the surface roughness is well approximated by a Gaussian distribution.

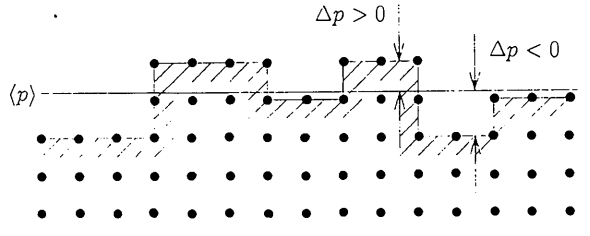


Fig. 5. A schematic illustration of $\langle p \rangle$ and Δp.

In practical applications of CTR scattering, however, it is a very useful result that the surface roughness can be obtained as the mean-square deviation of step height $\langle \Delta p^2 \rangle$ on an atomic level from the analysis of the CTR scattering for small q (Gibbs, Ocko, Zehner & Mochrie, 1988; Harada, Shimura, Takata, Yakushiji & Hoshi, 1990). The analysis proceeds in an analogous way to the determination of the thermal parameter from the Debye-Waller factor in ordinary crystal-structure analysis.

(iii) *Model calculation*

We see from (14) that the CTR intensity along the rod direction normal to the crystal surface decreases as $1/q^2$ for small q for an ideally flat surface and decreases more rapidly for a rough surface. Thus, the reduction of the observed intensity of CTR scattering from that calculated for an ideally flat surface at a certain q value enables us to estimate the mean-square deviation of step height, $\langle \Delta p^2 \rangle$. We may see how sensitive the CTR scattering is to the surface roughness by the model calculations based on (28), which are shown in Fig. 6, where the CTR scattering for several values of $\langle \Delta p^2 \rangle$ are compared. We see that the effect is especially pronounced for large values of q. The CTR scattering intensity for rough surfaces at $q = 0.2$ compared to that for the ideal surface is 72, 53 and 38% for $\langle \Delta p^2 \rangle = 0.2$, 0.4 and 0.6, respectively. These intensity reductions are readily observable with sufficient accuracy.

Once we have obtained the average value $\langle \Delta p^2 \rangle$ by the above method, we still have to answer the question: what lateral extent of the surface does the average represent? It does not depend obviously on the size of the incident X-ray beam but rather on the spatial coherency of the X-rays used in the experiment, if the crystal is perfect. However, it would be limited by the average size of the mosaic blocks of

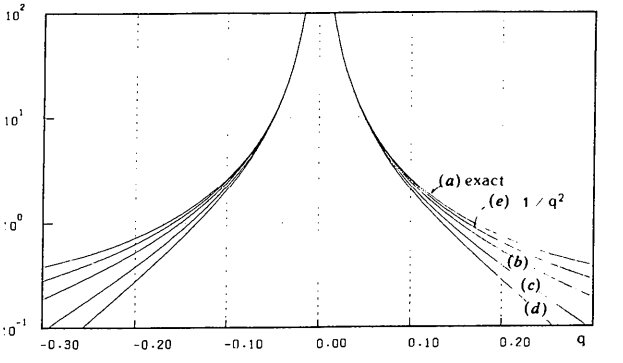


Fig. 6. Intensity change of the CTR scattering along the rod for several different degrees of surface roughness. (*a*) Ideal flat surface; (*b*), (*c*) and (*d*) rough surfaces with $\langle \Delta p^2 \rangle = 0.2$, 0.4 and 0.6 in Debye-Waller-like factor, respectively; (*e*) the $1/q^2$ relation, showing its deviation from the exact calculation (*a*) for the ideally flat surface.

crystals, if the crystal is not perfect. It means that the result depends both on the degree of perfection of the crystal used and on the optical system used in collimating the primary X-ray beam. It is rather difficult to estimate the range of the coherence, as the width of the CTR scattering is observed to be less than the instrumental resolution for the X-ray beam collimated by a double-crystal monochromator of Si in the parallel setting for the SR source BL-4C at the Photon Factory. However, Kashiwagura & Harada (1990) have estimated that it would be a few μm. This is in agreement with the value estimated as the temporal coherence length by Ishikawa (1990) on the basis of the nature of a SR source. Accordingly, we may say that the step height averaged over 10 μm^2 may be obtained by using the SR source.

Comparison with other formalisms

Another representation of the CTR scattering is to write the scattering amplitude in the form

$$F_{CTR}(K) = \sum_p \theta_p f \exp(iK_z pc) \times \sum_m \sum_n \exp[i(K_x ma + K_y nb)], \quad (29)$$

where θ_p is the probability of finding the atoms at the pth level from the surface. The meaning of θ_p is different from γ_p introduced in this paper. γ_p is defined as the probability of finding columns with a step height p on the surface. It represents the relative area of the terrace with step height p to the whole area of the surface, while θ_p shows the relative occupancy at the pth level. This relationship between γ_p and θ_p is illustrated in Fig. 7. We see from Fig. 7 that

$$\gamma_p = \theta_p - \theta_{p-1}. \quad (30)$$

(i) *Robinson's model*

In the analysis of the CTR scattering from the (111) Si wafer surface, Robinson (1986) introduced a single parameter β ($0 < \beta < 1$), representing the probability of finding atoms in a particular atomic layer. A schematic illustration of the surface region is shown in Fig. 8(a). θ_p is given by

$$\theta_p = \begin{cases} \beta^p & \text{for } p \geq 0 \\ 1 & \text{for } p < 0. \end{cases} \quad (31)$$

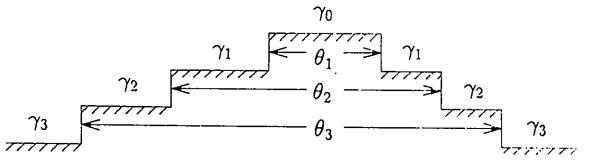


Fig. 7. An illustration of the difference between the definitions of parameters γ_p and θ_p: $\gamma_0 = \theta_0$; $\gamma_1 = \theta_1 - \theta_0$; $\gamma_2 = \theta_2 - \theta_1$ and so on.

By substituting (31) into (30), $|\Gamma(q)|^2$ is calculated as

$$|\Gamma(q)|^2 = (1-\beta)^2/[1+\beta^2-2\beta\cos(2\pi q)]. \quad (32)$$

This is the expression derived by Robinson (1986) for the damping factor for the CTR scattering.

(ii) *KKKH models*

Kashihara, Kawamura, Kashiwagura & Harada (1987) (referred to as the KKKH model) derived (29) by assuming that the distribution of atoms near the surface would have an exponential form, so

$$\theta_p = \begin{cases} 0 & \text{for } p > 0 \\ 1 - \eta \exp(p/\xi) & \text{for } p \leq 0, \end{cases} \quad (33)$$

where the two parameters $1-\eta$ and ξ represent the relative number of atoms at the top level of the surface and the characteristic depth of the surface roughness region, respectively. A schematic KKKH model is shown in Fig. 8(b). If we substitute (33) into (30) and calculate $\Gamma(q)$ from (14), we have

$$|\Gamma(q)|^2 = [1-\eta-(\eta-A)\exp(-2\pi iq)]^2 \times [1-A\exp(-2\pi iq)]^{-1} \quad (34)$$

where $A = \exp(-1/\xi)$. This corresponds to the damping factor for the KKKH expression. This expression has been used with success in the analysis of the surface morphology of several crystal surfaces (Kashihara *et al.*, 1987; Kashihara, Kimura & Harada, 1989; Kashihara *et al.*, 1991).

Comparison of the relations (32) and (34) shows that the relations become identical when we put $\eta = \exp(-1/\xi)$ in the KKKH model and also equate it to β in Robinson's model. Thus, an extreme case of the KKKH model is Robinson's model. At first the two density distributions along the direction normal to the surface are opposite to each other as seen from

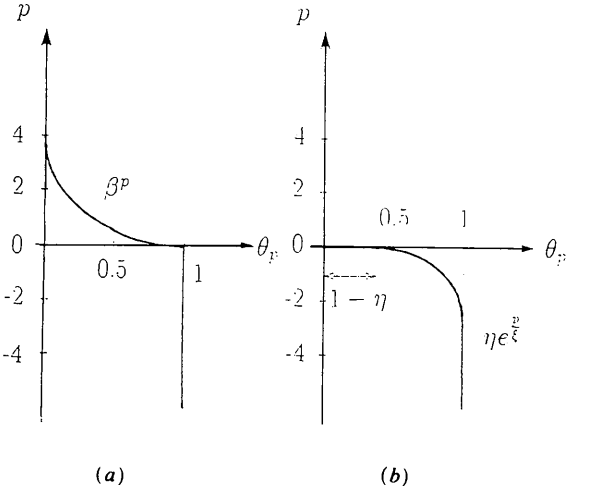


Fig. 8. A comparison of (a) Robinson's model and (b) the KKKH model. Depth p *versus* density θ.

Figs. 6(a) and (b), so that different answers are expected. But the same values of $|\Gamma(q)|$ are obtained for both models, as a consequence of the well known Babinet principle. In any models so far discussed the damping factor $|\Gamma(q)|^2$ for the CTR scattering can be represented in a Gaussian form of Debye–Waller-like factor, (26), for the small-q region.

Concluding remarks

In this paper, the effect of surface roughness on the X-ray CTR scattering has been discussed by developing a kinematical diffraction theory for the crystal with an extended surface. The theory is based on a simple orthogonal lattice, consisting of one atom in the unit cell. For real crystals the situation is not expected to be quite so simple. It is possible to extend the present theory for a lattice consisting of several atoms in the unit cell, without losing its generality, by simply replacing the atomic scattering factor f by the crystal structure factor F in (2) and (4). This replacement corresponds to taking a bunch of atomic chains starting from the atoms in the unit cell at the upper surface along the inward direction perpendicular to the surface. The summation will then be over the columns. However, the unit step height should be taken to be the length of the unit cell, if the present theory is adopted as it stands.

In general the surface of a real crystal is not as ideal as discussed here. Many kinds of steps with different step heights may exist on the surface that are not necessarily a multiple of the unit-cell height. Even in such cases, the present theory, in which the scattering is treated as that arising from a two-dimensional arrangement of column scatterers, could be extended by introducing multiple columns with different phases. An attempt at treating such cases has been recently described by Kashihara *et al.* (1991) in the study of the interface boundary of the GaAs (001) surface with an amorphous oxidized layer.

In this paper, we confined the discussion to the intensity profile along the CTR scattering, not the profile perpendicular to it or the diffuse scattering term. These subjects will be discussed in future papers.

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