Diffraction of x rays at the far tails of the Bragg peaks. II. Darwin dynamical theory

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The Darwin theory of dynamical diffraction by crystals is extended to include the regions between Bragg peaks as well as situations of grazing and normal angles of incidence, i.e., the whole angular range extending from 0° to 90°. The modified theory reproduces the usual two-beam Laue dynamical theory in the close vicinity of the Bragg peaks, while in the regions between the Bragg peaks it predicts reflectivities in agreement with the kinematical theory. Many-beam effects due to all crystallographic planes parallel to the surface can be calculated in an extremely simple way making this approach particularly suitable to artificial multilayered structures. The weak scattering in the region where the far tails of two neighboring Bragg peaks interfere contains information about the phases of the structure factors.

I. INTRODUCTION

X-ray-diffraction theories[1–4] are called either kinematical or dynamical depending on whether the effects of multiple scattering within the crystal are neglected or not. Thus, the predictions of the kinematical and the dynamical theories can be expected to agree if the scattered intensities are low. That this agreement holds is, in fact, well known in many situations.[1–4] One example is the case of Bragg reflections that are weak because the crystal is very thin or the structure factor is small. Another example, is the case of the relatively low intensity scattered *slightly* away (up to a few tenths of a degree) from Bragg peaks which may themselves be quite intense. In a previous paper[5] and in the present one, the issue is addressed of whether the agreement still holds *throughout* the region between two Bragg peaks, and not just in their immediate neighborhood. In contrast to the near-tail region mentioned above, in the far-tail region approximations which are normally made in the dynamical theory fail and have to be corrected.

The diffraction in the far tails of the Bragg peaks has practical interest in a number of important applications such as in the study of crystal surfaces[6,7] and in the problem of diffraction by artificial multilayered structures at grazing incidence.[8,9] In this latter case Bragg peaks are closely bunched together, and regions of high and low reflectivity, which exhibit either dynamical or kinematical behavior, alternate rapidly. A single theory applicable to both regimes is clearly desirable.

Most dynamical diffraction theories belong to one or the other of two rather broad groups. Theories in the first group essentially consist in solving for the self-consistent propagation of waves in periodic media. They originated in the work of Ewald and Laue.[1–3] Theories in the second group, originate with Darwin,[1,4,10] and approach the calculation of the reflected intensities by dividing the crystal as a stack of layers and explicitly considering the multiple scattering between different layers. (Some theories belong to both groups. For example, the basic equations of nuclear resonant diffraction[11] resemble Ewald's but the method of solution is Darwin's. Similarly, the differential equations of Takagi and Taupin[12] are deduced from Laue's phenomenological wave equation, but they relate the field amplitudes in successive *infinitesimal* layers, very much in the spirit of Darwin.) All of these theories involve approximations which are well justified under normal diffraction regimes but may demand special treatment in some cases. The improved approximations required to extend the regime of applicability of Laue's theory to the far tails of the Bragg peaks were the subject of the first paper in this series[5] and also of a paper by Colella.[7] The purpose of this second paper is to obtain analogous improvements for the Darwin theory.

The original Darwin theory[1,4,10] involves approximations which fail in the region between Bragg peaks, or for small angles of incidence close to the region of total external reflection, and also for Bragg angles near $\pi/2$.[13] Furthermore, only two-beam cases are considered; many-beam diffraction effects, which may be essential when Bragg peaks are spaced closely together, are normally neglected. The Darwin theory has been extended in several directions (to nuclear scattering,[11] to Laue transmission cases,[14] to asymmetric diffraction,[14,15] and using numerical matrix methods, to strained crystal surfaces and three-beam cases[15]), but the issue of the scattering in the far tails of the Bragg peaks has not so far been addressed.

In the theory offered here many of the usual approximations are avoided. Once we obtain the scattering and transmission of a single layer, the reflection and transmission coefficients of the crystal are calculated *without any further approximations.* This is done in Sec. II. This improved version of the Darwin theory offers significant simplification over the corresponding improved version of the Laue theory developed in the previous paper,[5] which has several complicating features such as the requirement of accurate knowledge of the dispersion surface, of the use of exact electromagnetic boundary conditions, and the limitation to a small number of beams. For example, full many-beam calculations (involving tens or perhaps even an infinite number of beams[9]) require only a very modest numerical effort.

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In Sec. III the scattering by a single atomic layer including many-beam effects is calculated using Fresnel diffraction theory. This is a kind of kinematical theory in the sense that multiple scattering within the layer is neglected. However, for grazing incidence intralayer multiple scattering effects may be appreciable: They are adequately accounted for by modifying the single-layer kinematical results to include the effects of absorption, refraction, and total external reflection. The proof that this version of the Darwin theory correctly describes both the close vicinity of the Bragg peaks and their far tails is given in Sec. IV. As a more practical application we address in Sec. V the problem of the diffraction by a thin layer on an otherwise perfect crystal. The nature of this layer is quite arbitrary, it may represent a rough, strained or reconstructed surface or even an oxide layer. Numerical results are given for a couple of idealized surface models. Final comments and conclusions are given in Sec. VI.

II. A MODIFIED DARWIN DYNAMICAL DIFFRACTION THEORY

A. The basic equations

The diffracting crystal considered here is in the shape of a plate, the surfaces of which are normal to the z direction, and the dielectric susceptibility is modeled by

$$\chi(\mathbf{r})=\sum_H \chi_H e^{i\mathbf{H}\cdot\mathbf{r}}=\sum_m \chi_m e^{2\pi imz/d} , \tag{2.1}$$

where $\mathbf{H}=2\pi m\hat{e}_z/d$, with m integer, are the reciprocal-lattice vectors. We deal only with diffraction in the symmetric Bragg case: The reciprocal-lattice vectors lie along the normal to the crystal surface (the z direction), and are those on the truncation rod passing through the origin in reciprocal space.

Let us imagine the crystal as built up of N layers of thickness d separated by small gaps (which will eventually be eliminated) of thickness 2ϵ (see Fig. 1). The fact that χ depends only on z and not on the transverse coordinates x and y implies that the components of the photon momentum along x and y are conserved. Therefore, only specular reflection occurs and the electric field in the nth gap is a superposition of "incident" and "reflected" plane waves,

$$\mathbf{E}(\mathbf{r})=(\hat{\epsilon}A_n e^{iq(z-nd)}+\hat{\epsilon}_R B_n e^{-iq(z-nd)})e^{iK\cos\theta x} , \tag{2.2}$$

where $K=\omega/c$ is the wave number in vacuum and

$$q=K\sin\theta , \tag{2.3}$$

is the component of the incident wave vector $\mathbf{K}$ tangential to the crystal surface. Notice that independently of the number of Fourier components appearing in Eq. (2.1), the exact field, Eq. (2.2), is a superposition of just two beams; this is important: An involved many-beam dynamical diffraction calculation, which can normally only be attacked numerically, reduces to what is essentially a simple two-beam calculation, which can be done analytically. In fact, one may even calculate cases which, in the conventional Laue approach, would involve an infinite number of beams.[9]

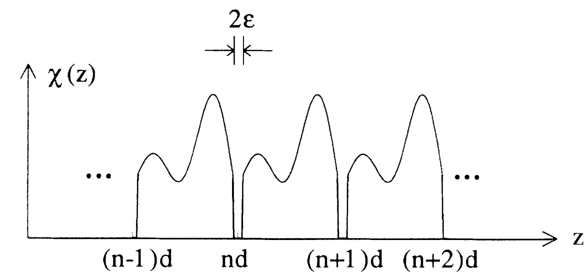

FIG. 1. The crystal is a sequence of N layers of thickness d and arbitrary profile separated by infinitesimal gaps.

Let r_1 and t_1 be the amplitude reflection and transmission coefficients of the single layer located between the gaps n and $n+1$, for an incident wave coming from $z=-\infty$ and propagating in the direction of increasing z, and let r_2 and t_2 be the corresponding coefficients for a wave propagating in the opposite direction. Then the amplitudes A and B at the nth gap are related to those in the $(n+1)$th gap by

$$A_n r_1 + B_{n+1} t_2 = B_n \tag{2.4a}$$

and

$$A_n t_1 + B_{n+1} r_2 = A_{n+1} . \tag{2.4b}$$

The requirement of crystalline periodicity is expressed by Bloch's theorem in the form

$$A_{n+1}=e^{ik_z d}A_n=e^{i(n+1)k_z d}A_0 \tag{2.5a}$$

and

$$B_{n+1}=e^{ik_z d}B_n=e^{i(n+1)k_z d}B_0 , \tag{2.5b}$$

where k_z is the z component of the crystal momentum. Substituting (2.5) into (2.4) leads to

$$A_n r_1 + (e^{ik_z d}t_2 - 1)B_n = 0 , \tag{2.6a}$$

$$(t_1 - e^{ik_z d})A_n + e^{ik_z d} r_2 B_n = 0 . \tag{2.6b}$$

In order that nontrivial solutions exist the determinant of (2.6) must vanish; this leads to a dispersion relation for k_z,

$$e^{ik_z^{\pm} d}=\{(1+t_1t_2-r_1r_2) \pm[(1+t_1t_2-r_1r_2)^2-4t_1t_2]^{1/2}\}\frac{1}{2t_2} . \tag{2.7}$$

Substituting (2.7) back into (2.6) we obtain values for the allowed amplitude ratios, $\rho_{\pm}=B_n/A_n$, which are

$$\rho_{\pm}=[Z\pm(Z^2-4r_1r_2)^{1/2}]\frac{1}{2r_2} , \tag{2.8a}$$

where

$$Z=1-t_1t_2+r_1r_2 . \tag{2.8b}$$

Therefore, the electric field (2.2) in the gaps is

$$\mathbf{E}_{\pm}(\mathbf{r})=e^{i(k_z^{\pm}z+K\cos\theta x)}\mathbf{\Phi}_{\pm}(z)\ , \tag{2.9a}$$

where the function $\mathbf{\Phi}_{\pm}(z)$ for z in the nth gap is given by

$$\mathbf{\Phi}_{\pm}(z)=A_0 e^{-ik_z^{\pm}(z-nd)}(\hat{\epsilon}e^{iq(z-nd)}+\hat{\epsilon}_R\rho_{\pm}e^{-iq(z-nd)})\ . \tag{2.9b}$$

Since $\mathbf{\Phi}_{\pm}(z)$ is periodic (the function $z-nd$ is periodic and $\rho_{\pm}$ is independent of n), the field $\mathbf{E}$ is explicitly of the form required by Bloch's theorem.

B. The semi-infinite crystal

To calculate the amplitude reflection coefficient r_D of a semi-infinite crystal we impose boundary conditions at the crystal surface. For $z<-\epsilon$, the field in vacuum is

$$\mathbf{E}(z)=\hat{\epsilon}e^{iqz}+\hat{\epsilon}_R r_D e^{-iqz}\ , \tag{2.10}$$

[where for notational convenience a factor $\exp(iKx\cos\theta)$ has been omitted], while for $-\epsilon<z<\epsilon$, the field in the 0th gap in the crystal is

$$\mathbf{E}(z)=A_0(\hat{\epsilon}e^{iqz}+\hat{\epsilon}_R\rho_{\pm}e^{-iqz})\ . \tag{2.11}$$

Notice that the boundary at $z=-\epsilon$ is a vacuum to vacuum interface. This makes the required boundary conditions very simple: continuity of the field and of its derivative at $z=-\epsilon$. Therefore $A_0=1$, and

$$r_D=\rho_{\pm}\ . \tag{2.12}$$

The reflectivity is given by

$$R_D=|r_D|^2\ . \tag{2.13}$$

The choice of sign in Eqs. (2.11) and (2.12) is determined by requiring that the net flow of energy be in the direction of increasing z, that is, into the crystal. In practice, this condition is very easy to implement: Choose the sign that leads to $R_D\le 1$.

C. The finite crystal

To calculate the amplitude reflection and transmission coefficients of a finite crystal composed of N layers we proceed as in the last section and impose boundary conditions at both the 0th and the Nth gap. For $z<-\epsilon$, the field in vacuum is given by (2.10), while for $z>Nd+\epsilon$, the field is

$$\mathbf{E}(z)=\hat{\epsilon}t_D e^{iqz}\ . \tag{2.14}$$

Within the crystal the field is a superposition of the two modes (2.9),

$$\mathbf{E}(z)=A_+e^{ik_z^+z}\mathbf{\Phi}_+(z)+A_-e^{ik_z^-z}\mathbf{\Phi}_-(z)\ . \tag{2.15}$$

The conditions of continuity of the field and its derivative at $z=-\epsilon$ and at $z=Nd+\epsilon$ lead to

$$1=A_++A_-\ , \tag{2.16a}$$

$$r_D=A_+\rho_++A_-\rho_-\ , \tag{2.16b}$$

$$t_D=A_+e^{i(k_z^+-q)Nd}+A_-e^{i(k_z^--q)Nd}\ , \tag{2.16c}$$

and

$$0=A_+\rho_+e^{i(k_z^+-q)Nd}+A_-\rho_-e^{i(k_z^--q)Nd}\ . \tag{2.16d}$$

Solving for r_D and t_D we obtain the desired results,

$$r_D=\frac{r_1}{r_2}\frac{(1-r_1/\rho_+)^N-(1-r_1/\rho_-)^N}{\rho_+(1-r_1/\rho_+)^N-\rho_-(1-r_1/\rho_-)^N}\ , \tag{2.17}$$

and

$$t_D=\frac{\rho_+-\rho_-}{t_2^N e^{iqNd}}\frac{(1-r_1/\rho_+)^N(1-r_1/\rho_-)^N}{\rho_+(1-r_1/\rho_+)^N-\rho_-(1-r_1/\rho_-)^N}\ . \tag{2.18}$$

Some details of the treatment above differ from the original Darwin theory.[1,4,10] For example, there are no explicit phase factors in Eq. (2.4); for "thick" mirrors with varying index of refraction it is more convenient to incorporate them into t_1 and t_2. The usual Darwin approach is to search for solutions of (2.4) of the form $A_n=\alpha^n\beta$ where α and β are constants which are not assigned any particular physical meaning; it is interesting that the Darwin *ansatz* $A_n=\alpha^n\beta$ is just Bloch's theorem. Finally, one should note again that the derivation of Eqs. (2.17) and (2.18) involves a restriction to reciprocal-lattice vectors of the form $\mathbf{H}=2\pi m\hat{e}_z/d$ with m any positive or negative integer. Having made this single restriction the treatment above proceeds without any further approximations: *Given the reflection and transmission coefficients of a single layer, the scattering by the crystal is calculated exactly.* In particular, the equations above are valid both close to and far from the Bragg peaks, and also for grazing, nongrazing or even normal incidence. Multiple scattering and many-beam interactions (as many beams as values of m are included in the calculation of the single layer scattering) are fully taken into account. This is important in situations where there are many Bragg peaks spaced closely together, as in the diffraction by multilayered structures at small Bragg angles.[9]

III. REFLECTION AND TRANSMISSION BY A SINGLE ATOMIC LAYER

When calculating the scattering by a single atomic layer in a crystal, multiple scattering events are unlikely (except perhaps at extremely grazing incidence) and may be neglected: A kinematical theory calculation should be a very good first approximation. One can then proceed to include some intralayer multiple scattering effects by correcting for refraction, absorption, and total external reflection. The amplitude reflection coefficient (including refraction and absorption corrections) is[5,9]

$$r_1=(1-e^{2iKd\sin\bar{\theta}})\left[\frac{-P}{4\sin\bar{\theta}}\sum_m\frac{\chi_m}{\sin\bar{\theta}-\sin\theta_m}\right]\ , \tag{3.1}$$

where

$$\sin\bar{\theta}\equiv(\sin^2\theta+\chi_0)^{1/2}\ . \tag{3.2}$$

θ_m is the Bragg angle corresponding to the vector $\mathbf{H}=2\pi m\hat{e}_z/d$. The factor P is 1 or approximately $\cos 2\theta$ depending on whether it is the electric or the magnetic field that is transverse to the plane of incidence (TE or TM polarization, respectively). The transmission coefficient is obtained in a similar manner by considering the electric field scattered in the forward direction. The result is

$$t_1=\exp(iKd\sin\bar{\theta}) \ . \quad (3.3)$$

The coefficients r_1 and t_1 refer to an incident wave coming from $z=-\infty$ and propagating in the direction of increasing z. We also need the coefficients r_2 and t_2 which refer to an incident wave coming from $z=+\infty$ and propagating in the direction of decreasing z: The reflection coefficient r_2 is obtained from r_1 by replacing χ_m by χ_{-m} and the transmission coefficient t_2 is equal to t_1 so that the subscripts 1 or 2 may be dropped.

For grazing incidence, close to the region of total external reflection ($\sin\bar{\theta}\simeq 0$), the reflectivity is high and the kinematical approximation above fails. This multiple scattering effect may be partially corrected by replacing the $m=0$ term in (3.2) and (3.3) by the correct Fresnel reflection and transmission coefficients of a homogeneous slab with susceptibility χ_0. To be specific, for TE polarization, these $m=0$ terms are

$$t_0=\frac{2\sin\theta\sin\bar{\theta}}{2\sin\theta\sin\bar{\theta}\cos(iKd\sin\bar{\theta})-(\sin^2\theta+\sin^2\bar{\theta})i\sin(iKd\sin\bar{\theta})} \quad (3.4a)$$

and

$$r_0=\frac{i\chi_0\sin(iKd\sin\bar{\theta})}{2\sin\theta\sin\bar{\theta}}\frac{1}{t_0} \ . \quad (3.4b)$$

The expressions for r_D and t_D given in Sec. II when supplemented by the single layer coefficients given in this section provide a full solution to the diffraction problem. Notice, in particular, the ease with which many-beam dynamical effects are taken into account: Just include more terms in the summation (3.1) for the single layer kinematical reflection coefficient.

IV. LIMITING FORMS

Now we show that the modified Darwin theory of the previous sections reproduces the usual two-beam Laue dynamical theory in the close vicinity of the Bragg peaks, while in the regions between the Bragg peaks it predicts reflectivities in agreement with the kinematical theory.

In the vicinity of a given Bragg peak $\sin\bar{\theta}\simeq\sin\theta_n$. Using

$$\frac{e^{2iKd(\sin\theta_n-\sin\theta_m)}-1}{Kd(\sin\theta_n-\sin\theta_m)}=2i\delta_{mn} \ , \quad (4.1)$$

one obtains

$$r_1\simeq\frac{in\pi}{2\sin^2\theta_n}P\chi_n \ . \quad (4.2)$$

For r_2 a similar expression holds with χ_n replaced by χ_{-n}. The calculation of t requires more care: For $\sin^2\theta\gg\chi_0$ we have

$$\sin\bar{\theta}\simeq\sin\theta+\frac{\chi_0}{\sin\theta_n} \ , \quad (4.3)$$

so that, from Eq. (3.3)

$$t^2\simeq 1+\frac{in\pi z}{\sin^2\theta_n} \ , \quad (4.4)$$

where

$$z=\chi_0-2\sin\theta_n(\sin\theta_n-\sin\theta) \quad (4.5)$$

is the usual incidence variable z of the two-beam Laue theory [see Eq. (2.20) of Ref. 5]. Thus, Eq. (2.8b) becomes

$$Z\simeq-\frac{in\pi z}{\sin^2\theta_n}+O(\chi^2) \ . \quad (4.6)$$

Substituting (4.2) and (4.6) into (2.8) we get

$$\rho_{\pm}=[-z\pm(z^2-P^2\chi_n\chi_{-n})^{1/2}]\frac{1}{P\chi_{-n}} \ , \quad (4.7)$$

which is precisely the amplitude ratio as given by the Laue dynamical theory [Eq. (2.21) of Ref. 5]. Thus, in the close vicinity of the Bragg peaks the modified Darwin reflectivity (2.13) reproduces the Laue result.

It is only very close to the Bragg peaks that the phase factor $t=\exp(iKd\sin\bar{\theta})$ is close to 1 and the variable Z is small. Far from the Bragg peaks the quantity Z is much larger, in fact, $Z^2\gg 4r_1r_2$. Then

$$\rho_-\simeq\frac{r_1}{Z}\simeq\frac{-P}{4\sin\bar{\theta}}\sum_m\frac{\chi_m}{\sin\bar{\theta}-\sin\theta_m} \ , \quad (4.8)$$

and the reflectivity of a semi-infinite crystal [Eqs. (2.12) and (2.13)] turns out to be identical to the kinematical result [Eq. (2.6) of Ref. 5]. For a finite crystal the proof is equally simple. Using the identity

$$\rho_+\rho_-=\frac{r_1}{r_2} \quad (4.9)$$

and (4.8), we have

$$\rho_+\simeq\frac{Z}{r_2}\gg\rho_- \ . \quad (4.10)$$

Then, Eq. (2.17) becomes

$$r_D\simeq\rho_-(1-t^{2N}) \ , \quad (4.11)$$

which is, again, identical to the kinematical expression.

V. SCATTERING BY A THIN LAYER ON THE SURFACE OF A CRYSTAL

The reflectivity of the crystal substrate covered with a thin surface layer is given by

$$R \simeq |r_D + r_{SL}|^2 , \tag{5.1}$$

where the origin of coordinates has been chosen at the substrate surface so there are no additional phase factors, r_D is given by Eq. (2.12), and r_{SL} is the reflection coefficient of the layer. For sufficiently thin layers r_{SL} may be calculated using the same Fresnel kinematical theory used for the perfect crystal single layer.[5,9]

As a specific numerical example we consider the diffraction of Cu $K\alpha$ radiation by a semi-infinite perfect silicon crystal the surface of which is normal to the [111] direction. Figure 2 shows the reflectivity for the sharply terminated ideal surface for *incidence angles covering the full range from* 0° *to* 90°. The calculation includes all 11 beams of the form (h,h,h) for $h=0,\pm1,\ldots,\pm5$. For the nearly forbidden (222) reflection we use the value[16] $f_{222}=-0.169$. We find that although the reflections $(\bar{1}\bar{1}\bar{1})$ and (555) do not show up as sharp Bragg peaks in the range from 0° to 90°, their tails make very appreciable contributions to the intensity in the regions of low and high angles.

Figure 2 also shows the reflectivity for two idealized models of nonsharply terminated surfaces. For the first model the susceptibility $\chi_{SL}^{(1)}(z)$ of the surface layer vanishes for $z>0$ and for $z<0$ is given by the perfect crystal form, Eq. (2.1), multiplied by a smooth exponential decay $e^{z/\alpha d'}$:

$$\chi_{SL}^{(1)}(z) = \sum_m \chi_m e^{2\pi i m z/d'} e^{z/\alpha d'} . \tag{5.2}$$

The layer lattice spacing d' need not necessarily coincide with the substrate spacing d. For the second model we choose a form that is perhaps slightly more realistic: $\chi_{SL}^{(2)}(z)$ vanishes for $z>0$ and for $z<0$ is given by the perfect crystal form Eq. (2.1) multiplied by a stepwise exponential, i.e., for $-Nd'<z<-(N-1)d'$ we have

$$\chi_{SL}^{(2)}(z) = \sum_m \chi_m e^{2\pi i m z/d'} e^{-N/\alpha} . \tag{5.3}$$

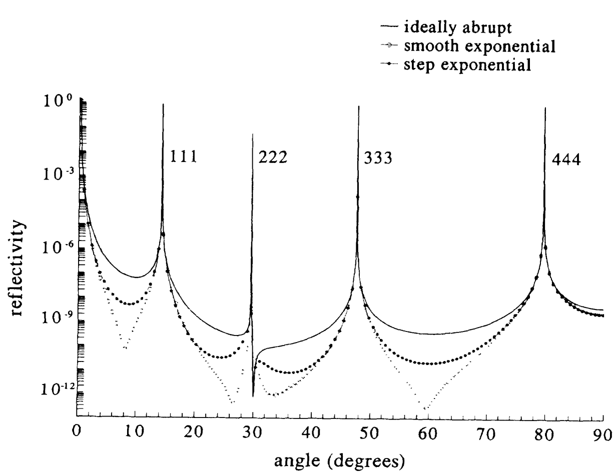

FIG. 2. The reflectivity of a silicon crystal cut along the 111 planes for three idealized surfaces structures (abrupt termination, exponentially smooth, and stepwise exponential terminations).

In both cases α measures the $1/e$ decay distance in units of d'. The corresponding kinematical amplitude reflection coefficients are

$$r_{SL}^{(1)} = \frac{1}{4\sin\theta} \sum_m \frac{P\chi_m}{\sin\theta - \sin\theta_m - i/2K\alpha d'} , \tag{5.4}$$

and,

$$r_{SL}^{(2)} = \frac{1-e^{2iKd'\sin\theta}}{1-e^{2iKd'\sin\theta}e^{1/\alpha}} \frac{1}{4\sin\theta} \sum_m \frac{P\chi_m}{\sin\theta - \sin\theta'_m} , \tag{5.5}$$

where θ'_m are the Bragg angles corresponding to d'. The calculations in Fig. 2 are for $\alpha=2$ and $d=d'$. Two interesting features are, first that sharper boundaries lead to higher scattered intensities between the Bragg peaks, in agreement with previous work.[6] And second, the sharp dip in reflectivity on the high angle side of the 222 reflection which originates in the destructive interference between the tails of the 222 and 333 reflections. The dip is very close to the 222 peak because this is a very weak reflection; one can check that artificially increasing $|f_{222}|$ shifts the dip to the right.

Thus, we see that the scattering in the far tails of the Bragg peaks contains information not just about the surface structure but also about the relative phases of the structure factors of neighboring Bragg peaks.

VI. SOME FINAL REMARKS AND CONCLUSIONS

The range of applicability of the Darwin theory of dynamical diffraction has been extended to include the regions between Bragg peaks as well as grazing and normal angles of incidence. The modified theory reproduces the usual two-beam Laue dynamical theory in the close vicinity of the Bragg peaks, while in the regions between the Bragg peaks it predicts reflectivities in agreement with the kinematical theory. An interesting feature, which should make this theory particularly convenient to describe the diffraction of artificial multilayered structures, is that many-beam effects can be calculated in a very simple way.

Although we have dealt with diffraction in the symmetric Bragg case, the improved dynamical approximations obtained here can be employed, using the method described by Borie,[14] in more general cases such as asymmetrical Bragg cases, or Laue cases, or even to other nontruncation rod many-beam cases. Unfortunately, in these cases, the ease with which many-beam effects can be calculated is lost. Likewise, our improved approximations can be incorporated into the theories of Hannon and Trammel,[11] Takagi and Taupin,[12] Berreman and Macrander,[15] and also to the case of grazing incidence diffraction[17] of Afanaseev and Melkonyan and of Jach *et al.* The reason these theories did not directly apply to the far-tail region is not due to any intrinsic shortcoming in the formalism but rather that these authors developed approximations specific to the problem of their immediate interest, namely the Bragg peaks themselves.

Finally, we found that the weak scattering where the far tails of two Bragg peaks interfere contains information about the phases of structure factors. For semi-infinite perfect crystals the scattering is very weak due to almost complete destructive interference between the various crystal planes. On the other hand in artificial multilayered structures the scattering in the far tails is readily observable and known to contain phase information.[18] An interesting question is whether such a method can be extended to small or imperfect crystals, for which destructive interference is not nearly as complete, and which are precisely the kind of crystals for which phase determination is still an interesting problem.

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