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Bragg Law and Darwin Model of Scattering Upon Inclusion of Ewald Self-Consistency Principle

by

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A scattering unit concept is used to solve Maxwell's equations for a Darwin-type model of a crystal. The latter is taken to be a stack of identical and equally spaced dipole planes. The self-consistent solution obtained for one of the planes is extended to series of planes representing the whole crystal. The solution obtained in closed-form, depends upon: a) continuity of all vectors which define the EM field between the adjoining units and b) geometric similarity of EM fields which activate the dipoles at different planes. Once both conditions are satisfied they bring about: the modified Bragg law and a hyperbola relating phase-shifts of both waves equivalent to the main equation of the dynamic theory. While the model is a development upon that of Darwin, the two divergent points from his model are: a) vectorial waves are used to define the EM field instead of scalar waves. b) interaction of all dipoles within the same plane is taken into account, wherein the principle of energy conservation is obeyed. Our model accepts: i) an imperfect upper crystal surface, ii) the second incident wave at the lower crystal surface may be of arbitrary amplitude and phase, iii) periodicity deviations due to the thermal motion or defects, iv) any actual crystal size (small or big).

Key-words: Bragg law; Darwin model; Ewald self-consistency principle.

I. INTRODUCTION

There have been developed historically, three formulations of the dynamic theory to account for the X-ray diffraction patterns from perfect crystals. The first phenomenological theory given by Darwin[1] takes advantage of the same complex amplitude summation carried out by the formalism of the Fourier transform but effected within the crystal space, rather than at a far away distance, such as required by the plane wave model. The second theory, due to Ewald[2], solves Maxwell's equations for a periodic array of classical dipoles under the *self-consistency principle*, in which polarization at a given dipole depends upon the polarization of the other dipoles within the crystal as well as the external field [see Slater[3]]. This second theory was extended by vonLaue[4] for a medium of periodic, continuous and complex dielectric constant into the most generally used form. In this extension, however, the theory assumed a macroscopic aspect and the Ewald's self-consistency principle lost its original and exact meaning. According to Kato[5], each of these three branches of the dynamic theory offers some attractive points and so may be used at one's preference. Such a wealth of theoretical tools, however, seems to be yet not adequate as shown by many examples of the diffraction profiles analysis where dynamic-type arguments are applied to the main body of the diffraction peak and the kinematic ones to its slopes.

We propose a new approach to the X-ray crystal scattering in which the Darwin model of scattering is a reference base, the Hertz vector method is the main instrument of calculation and the Ewald self-consistency principle is rigorously applied. By applying the formalism, which has already been developed for the scattering unit (Keller[6]; here called paper II), and requiring the geometric similarity of the EM fields we are able to reproduce results obtained by the customary dynamic theory for the symmetric Bragg case with substantially new information. These results, evolve into those obtained by means of the Fourier transform continuously linking the two formally different X-ray theories (dynamic and kinematic) into one common approach. The theory is valid for big perfect crystals, for small ones and for imperfect ones.

II. CRYSTAL MODEL

The model used for calculations is essentially the Darwin model of scattering in a situation when the cross-grating diffraction effects become of no importance and when only the two interacting waves have to be considered. In this case it is reasonable to assume a continuous and constant distribution of the scattering electrons over all those planes which are normal to the actual diffraction vector[7]. Since scattering electrons behave as classical harmonic oscillators we consider the latter planes as filled up by induced dipoles with a surface density equal to that defined for electrons.

To take advantage of the formalism worked out in paper II for a single plane of dipoles we assume a discrete ordering of these latter. Accordingly, the crystal model is supposed to be a stack of equally spaced and identical dipole planes. One of these planes together with a neighboring free space, filled up by the propagating field of the two incident and two transmitted waves, is considered a *scattering unit.* The above model, equivalent to regarding the crystal as formed by point-like atoms, one for each unit cell, will be reconsidered later in order to take into account the actual content of the unit cell and the actual shapes of the constituent atoms.

A field propagating within the unit, called *mesofield* in paper II, is in the self-consistent interaction mode with a stationary field formed by the two incident waves and the contribution due the oscillating dipoles termed *epifield.* Both above concepts[8] have no relation with those used in Ewald's papers. It will soon be evident that there is neither need nor place to include them into the present model.

The main conclusions reached in paper II were:

- the dipole contributions take the shape of two EM plane waves which are formed immediately after the take off,
- they leave symmetrically the scattering plane with an angle equal to that of the incident wave,
- the scattering of the two EM waves by a plane of dipoles can be decomposed into two independent vibrations; normal σ and parallel π to the incidency plane,
- the self-consistent solution cannot admit any wave that would leave the scattering plane at any other directions than those two defined by incident waves. This makes the scattering of two EM plane waves by the plane of dipoles an exclusively two-beam case.

The customary dynamic theory regards EM wave-field within the entire crystal space as a single entity. Here, a space assigned to the eventual solution is actually reduced to that occupied by a single unit. The unit frames the smallest element of space within which a solution for the EM field is actually obtained and all its properties determined. Within this space of the unit the two interacting waves are coherently coupled with energy being swapped between them under a strict conservation of energy regime.

The boundary conditions applied here are, in consequence, much more stringent than those which usually appear in the customary dynamic theory. Continuity of the EM field with regard to polarization and wave vectors must be rigorously observed at all the boundary planes. This equally refers to the internal planes between the adjoining units as well as to the two external ones which are delineating the entire model space.

A demand of the 'internal' boundary conditions for all scattering units makes the all-important crystallographic feature of periodicity, in a way, redundant. This fact brings about some consequences of a real practical importance. On one hand, it enables one to treat X-ray scattering from layered structures of special type and, on the other, to analyze the scattering models over a complete range ($0 - 90$ deg) of the angles Θ. Accordingly, the treatable layer structures can come from various crystal substances and be defined by variable plane numbers. Thus, the present approach seems best suited for the diffraction studies on superlattices and multilayer structures.

III. MODELS AND SOLUTIONS

Since crystal periodicity is no more a sine qua non condition in order to obtain rigorous solutions for an extensive class of scattering models it becomes useful to use a 'periodicity degree' of the model only as a criterion to classify all possible solutions for layer structures of different kinds. These latter, obtained without exception numerically, in some particular cases can be developed into suitable analytical formulas.

At one extreme, we have a model of zero periodicity-degree composed by a set of dipole planes defined by variable dipole densities and spacings. Naturally, the model gives up a projection of the unit cell content on actual diffraction vector and the derived solution will contain in some form the structure factor. This solution will be termed a *general* type.

At the other extreme, we consider a set made of equidistant and equal dipole planes. Likewise, the model gives up projection of a perfect crystal structure on the mentioned diffraction vector and the solution, for some particular values of incidence angle, should result in the modified Bragg equation. Accordingly, this solution will be conveniently called a *Bragg* type.

Somewhere in between the two extremes, a holistic image of self-consistent X-ray scattering in the symmetric Bragg case valid for perfect crystals, superlattices and multilayer structures, is obtained.

In order to complete the list of solutions we should state that the Bragg type solution as a function of the boundary conditions can assume two distinct forms. The first one, defined by a certain demand on the EM field to be specified later, will be conveniently called an *infinite* solution. The other one will be termed a *finite* solution. The latter includes an important case of a *real* solution.

A significance of the names proposed will be made clear by a more detailed approach in the following sections.

IV. GENERAL SOLUTION

A procedure to obtain the general solution is a trivial one. From paper II we recall that a function of the scattering unit is completely given by its matrix. In the same way this function for a set of such units is defined by the resultant matrix obtained as a product of respective matrix-components while taking into account the continuity of all the polarization and wave vectors which define the EM field between the adjoining units.

Calculations will be carried out by means of the notation used in paper II. Hence, dipole planes are planes defined by a sequence of equations $x = x_k$, with $x_k > 0$ and $k = 1, ..., K$ and where K is a total number of dipole planes. The first plane is defined by plane $x_1 = 0$. We recall that dipole planes of the model are uniformly filled by the scattering electrons which vibrate as classical harmonic oscillators without energy loss. The surface density of electron distribution within the dipole planes of the model is described by a sequence of real numbers σ_k.

We assume that two harmonic plane EM waves of an arbitrary elliptical polarization A_k^{in} and B_k^{in} are symmetrically incident on each dipole plane at a general angle θ. The polarization vectors of electrical parts of these two waves are given by

$$\left.\begin{array}{l}\vec{\mathbf{E}}^{in}_{\mathrm{Ak}}(\vec{\mathbf{r}},t)=(\vec{\mathbf{A}}^{in}_{\pi k}+\vec{\mathbf{A}}^{in}_{\sigma k})\,\exp[\,i(\omega t-\vec{\mathbf{k}}^{in}_{\mathrm{A}}\cdot\vec{\mathbf{r}})\,]\\ \vec{\mathbf{E}}^{in}_{\mathrm{Bk}}(\vec{\mathbf{r}},t)=(\vec{\mathbf{B}}^{in}_{\pi k}+\vec{\mathbf{B}}^{in}_{\sigma k})\,\exp[\,i(\omega t-\vec{\mathbf{k}}^{in}_{\mathrm{B}}\cdot\vec{\mathbf{r}})\,]\end{array}\right\}\ \text{where}\ \left\{\begin{array}{l}\vec{\mathbf{k}}^{in}_{\mathrm{A}}=k\,[\ \ \sin\theta,\cos\theta,0]\\ \vec{\mathbf{k}}^{in}_{\mathrm{B}}=k\,[-\sin\theta,\cos\theta,0]\end{array}\right. \quad (1)$$

are wave vectors with magnitudes $k = 2\pi/\lambda$ of the incident waves A_k^{in} and B_k^{in}, respectively. Space coordinates are given by $\vec{r}_k = [x - x_k, y, z]$. The polarization vector components parallel to the incidence plane are denoted by $\vec{\mathbf{A}}^{in}_{\pi k}$ and $\vec{\mathbf{B}}^{in}_{\pi k}$ while the components normal to it are given by $\vec{\mathbf{A}}^{in}_{\sigma k}$ and $\vec{\mathbf{B}}^{in}_{\sigma k}$. Each of these vector components may be represented as a product of a complex amplitude which includes a phase and a respective versor indicating direction of vibration as follows:

$$\begin{aligned}
&\vec{\mathbf{A}}^{in}_{\pi k}=\mathbf{A}^{in}_{\pi k}\hat{\mathbf{e}}_{\pi A},\quad \mathbf{A}^{in}_{\pi k}=|\mathbf{A}^{in}_{\pi k}|\exp(i\alpha^{in}_{\pi k}),\quad \hat{\mathbf{e}}_{\pi A}=[\cos\theta,-\sin\theta,0],\\
&\vec{\mathbf{A}}^{in}_{\sigma k}=\mathbf{A}^{in}_{\sigma k}\hat{\mathbf{e}}_{\sigma A},\quad \mathbf{A}^{in}_{\sigma k}=|\mathbf{A}^{in}_{\sigma k}|\exp(i\alpha^{in}_{\sigma k}),\quad \hat{\mathbf{e}}_{\sigma A}=[0,0,1],\\
&\vec{\mathbf{B}}^{in}_{\pi k}=\mathbf{B}^{in}_{\pi k}\hat{\mathbf{e}}_{\pi B},\quad \mathbf{B}^{in}_{\pi k}=|\mathbf{B}^{in}_{\pi k}|\exp(i\beta^{in}_{\pi k}),\quad \hat{\mathbf{e}}_{\pi B}=[\cos\theta,+\sin\theta,0],\\
&\vec{\mathbf{B}}^{in}_{\sigma k}=\mathbf{B}^{in}_{\sigma k}\hat{\mathbf{e}}_{\sigma B},\quad \mathbf{B}^{in}_{\sigma k}=|\mathbf{B}^{in}_{\sigma k}|\exp(i\beta^{in}_{\sigma k}),\quad \hat{\mathbf{e}}_{\sigma B}=[0,0,1].
\end{aligned} \quad (2)$$

Step-like changes of their amplitude and phase in relation to the incident waves are included in their respective complex amplitudes, modified after each scattering event. These waves result from the scattering unit solution which in the first step defines the self-consistent dipole vibrations, and then the amplitudes of the transmitted waves.

Since the two kinds of vibrations of π- and σ-polarization are shown to be independent of one another, in the following we will present only the more complex formulas for the π-polarization state.

The scattering unit solution as given in a matrix equation form in paper II (eq. 27) is valid for each k-th dipole plane separately defining the amplitudes of the two scattered forward (or better, transmitted) waves A_k^{tr} and B_k^{tr} in function of the amplitudes of the two incident waves A_k^{in} and B_k^{in}.

However, it can be better to define another relationship, namely, between the amplitudes of the *mesofield* acting *above* the k-th scattering dipole plane (superscript a) and represented by a matrix of dimension 2×1

$$\mathcal{M}_k^a = [\mathbf{A}_k^{in}, \mathbf{B}_k^{tr}] \tag{3}$$

and the respective amplitudes of the *mesofield* which appears *below* this plane (superscript b) defined by a similar matrix of the same dimension

$$\mathcal{M}_k^b = [\mathbf{A}_k^{tr}, \mathbf{B}_k^{in}]. \tag{4}$$

This can be independently done for both states of polarization. After an algebraic reformulation to include also the free space environment for each of the dipole planes and the notation complemented by the subscript k we obtain a new equation much more suitable for treatment of the stack of dipole planes

$$\mathcal{M}_k^a = \mathbf{M}_{pk} \cdot \mathcal{M}_k^b, \tag{5}$$

where $\mathbf{M}_{pk}$ represents a new matrix of dimension 2×2 defining scattering properties of a *primitive* (single) plane of dipoles termed accordingly *primitive scattering matrix.* Its elements in an explicit form are

$$\mathbf{M}_{pk} = (\cos\varepsilon_{\theta k})^{-1} \begin{bmatrix} \exp[+i(\delta_k - \varepsilon_{\pi k})] & i\sin\varepsilon_{\theta k} \\ -i\sin\varepsilon_{\theta k} & \exp[-i(\delta_k - \varepsilon_{\pi k})] \end{bmatrix}; \tag{6}$$

where δ_k represents a phase factor due to a path difference between the adjoining units. The above notation corresponds to a situation where the dipole plane is located at a center of each unit at $x = x_k + d_k/2$ and each unit space is framed by the x coordinate confined within a semi-closed interval $(x_k, x_{k+1}]$ where $x_{k+1} = x_k + d_k$, $\delta_k = k\, d_k \sin\theta$ with d_k representing a distance between the $k+1$-th and k-th dipole planes.

In the case of the σ-polarization the two angles $\varepsilon_{\pi k}$ and $\varepsilon_{\theta k}$, valid for π-polarization, are replaced by the single angle $\varepsilon_{\sigma k}$. All three are given by

$$\begin{aligned} \varepsilon_{\pi k} &= \arctan\{f_{pk} / [1 - (f_{pk}\sin 2\theta)^2/4]\}, \\ \varepsilon_{\theta k} &= \arctan\{f_{pk} / [1 + (f_{pk}\sin 2\theta)^2/4]\}, \\ \varepsilon_{\sigma k} &= \arctan f_{pk} \end{aligned} \tag{7}$$

where $f_{pk} = r_e \sigma_k \lambda / \sin\theta$ is the introduced *scattering factor of the k-th dipole plane,* defined by the classical electron radius r_e, the radiation wavelength λ and the incidence angle θ, all constant for the whole model, and the surface density of electron distribution σ_k which can vary from one k-th dipole plane to another.

We note that the new matrix just obtained has two important properties:

- it is unimodular,
- the matrix elements are complex conjugate on both diagonals.

A general solution for the scattering model is obtained recalling the self-consistency principle represented for each k-th primitive scattering unit by the matrix (6) and demanding a continuity of the mesofield between all adjoining units. The continuity condition means that transmitted waves A_k^{tr} from an upper primitive scattering unit become incident waves A_{k+1}^{in} for a lower one and the same procedure is repeated for waves B_{k+1}^{tr} and B_k^{in}, respectively. This condition has to be independently valid for both states of polarization and for all the internal boundary planes $k = 1, \ldots, K-1$ with K a total number of primitive scattering units. It reads in terms of the accepted mesofield notation as:

$$\mathcal{M}_k^b \equiv \mathcal{M}_{k+1}^a. \tag{8}$$

The general solution obtained under both self-consistency (5) and continuity (8) conditions can be written in a matrix form as follows:

$$\mathcal{M}_{a1} = \mathbf{M}_u \cdot \mathcal{M}_{bK}, \quad \text{where} \quad \mathbf{M}_u = \prod_{k=1}^{K} \mathbf{M}_{pk} = \begin{bmatrix} a_u & b_u \\ c_u & d_u \end{bmatrix} \tag{9}$$

a resultant matrix of dimension 2×2 valid for any scattering model can be appropriately called, depending on application, a *general scattering matrix* or *unit scattering matrix*. Its matrix elements can be given in an explicit way in the form of series.

In fact, if the scattering model represents a projection of the unit cell structure, the two elements b_u and c_u of the scattering matrix (9) contain the kinematic structure factor for the front and back reflection from the non-primitive unit cell, respectively. It may be given in an explicit way and compared with this factor while disregarding some higher terms in the series.

The matrix formulation of the general scattering problem enables one to see that the solution obtained for a set of scattering planes is not really different from that derived for a single dipole plane. Both include respective matrices which transform the complex amplitudes of the mesofield below the scattering model into the corresponding ones of the mesofield above it. Both solutions depend exclusively on the structure itself and not on the EM field surrounding the structure.

In consequence, it is possible to extend the single scattering unit solution to one which is valid for a crystal. It is represented by the unit scattering matrix (9) and continuity conditions which refer now to the internal boundary condition between the adjoining non-primitive scattering units. Again in terms of the mesofield notation it reads

$$\mathcal{M}_j^b \equiv \mathcal{M}_{j+1}^a. \tag{10}$$

which the subscript j enumerates the EM field solutions which, in spite of the fact that all the scattering units are identical, does not need to be necessarily the same for each. It changes as $j = 1, \cdots, J-1$ where J determines the total number of the scattering units in the model.

The crystal solution obtained can be also given as follows

$$\mathcal{M}_1^a = \mathbf{M}_c \cdot \mathcal{M}_J^b, \quad \text{where} \quad \mathbf{M}_c = \prod_{j=1}^{J} \mathbf{M}_u = \begin{bmatrix} a_c\, b_c \\ c_c\, d_c \end{bmatrix} \tag{11}$$

where matrices $\mathcal{M}_1^a$ and $\mathcal{M}_J^b$ represent now 'external' mesofield above and below the crystal, respectively. The *crystal scattering matrix* $\mathbf{M}_c$ of dimension 2×2 is obtained as a product of the J identical single unit scattering matrices given before. The elements of the crystal scattering matrix will be expressed in terms of those of the unit scattering matrix by means of the Chebyshev polynomials in section 8. The solution obtained by help of the crystal scattering matrix may be given in a more explicit form as

$$\begin{bmatrix} \mathbf{A}_{11}^{in} \\ \mathbf{B}_{11}^{tr} \end{bmatrix} = \begin{bmatrix} a_c\, b_c \\ c_c\, d_c \end{bmatrix} \cdot \begin{bmatrix} \mathbf{A}_{KJ}^{tr} \\ \mathbf{B}_{KJ}^{in} \end{bmatrix} = \begin{bmatrix} a_u\, b_u \\ c_u\, d_u \end{bmatrix}^J \cdot \begin{bmatrix} \mathbf{A}_{KJ}^{tr} \\ \mathbf{B}_{KJ}^{in} \end{bmatrix}. \tag{12}$$

Resuming, in the all analyzed cases the respective scattering matrix can be regarded as time-reversible EM field operator which transforms the two propagating waves below the scattering model, into the corresponding ones above it or vice versa. In the latter case the solution is obtained by help of an inverse operator defined by a matrix which is in an inverse relation to the respective scattering matrix.

We note also that the same developed procedure is applicable to solving the scattering problems in the multilayer structures and superlattices.

V. REAL SOLUTION

A real case solution represents a subset of the general solution (12) in the absence of the second incident wave at the lowest dipole plane in the stack: $\mathbf{B}_{KJ}^{in} \equiv 0$. We will take the amplitude of the first incident wave to be normalized according to $\mathbf{A}_{11}^{in} \equiv 1$ for both polarization states which leads to definition of the transmission $\mathcal{T}_c^J$ and reflection $\mathcal{R}_c$ coefficients resulting from a particular form of the equation (12):

$$\begin{bmatrix} 1 \\ \mathcal{R}_{cJ} \end{bmatrix} = \begin{bmatrix} a_c\, b_c \\ c_c\, d_c \end{bmatrix} \cdot \begin{bmatrix} \mathcal{T}_{cJ} \\ 0 \end{bmatrix}. \tag{13}$$

In the course of the numerical solution we note that below the lower crystal boundary propagates only one transmitted wave for which we assume first its complex amplitude equal to 1. Then, by help of the crystal scattering matrix we derive the two complex amplitudes of both incident and reflected beams above the upper boundary. Finally, we transfer the normalization condition to the amplitude of the incident beam.

The above method for obtaining the amplitudes of the transmitted and reflected waves is quite general and, as can be noted, does not depend on periodicity of the model. On the other hand, taking into account that even for a crystal model its periodicity does not necessarily refer to the EM field itself, it will be useful to enumerate solutions obtained for the different scattering units.

It turns out that it is more useful to deal not with the complex amplitudes of the respective waves but rather with their appropriately chosen ratios. These latter, conveniently called *factors*, refer to the same or different beams and will be defined according to necessity for a single dipole plane, a scattering unit or a conveniently chosen set of units. Since the introduced factors depend, in general, on a 'depth' within the crystal we assume for them the name *local*. Jointly these factors will serve to carry out a complete mapping of the entire EM field on the atomic or 'microscopic' level.

In some particular cases of the periodic structures the introduced factors may assume the same numerical values for all units of the model and the solution obtained assumes a macroscopic aspect. It can be given in an analytic form while the factors themselves will be accordingly called the *global* ones.

In another most important case of a real situation the above factors are practically periodic throughout a substantial part of the model and they are not in that part which is neighboring its lower boundary. In other words, we note an effect of the wave field convergence which by itself deserve a separate treatment.

VI. WAVE FIELD CONVERGENCE

The convergence effect in the wave field formation can be regarded as one of the most significant diffraction phenomena which is usually and most unfortunately overlooked in the customary approach. The careful analysis of this effect will lead to two important conclusions:

- the overall diffraction effect results from only those structural elements which are statistically repetitive throughout the main body of the scattering structure,
- a perfect boundary surface has for the planar model of structure only a secondary importance.

In order to analyze the convergence problem we will take advantage of the factors introduced in paper II (eqs. 31, 33, 36) which all depend on the structure via the angles ε_π and ε_θ and on the incident mesofield given by

$$\mathcal{F}_{\pi j} = f_{\pi j} \exp(i\varphi_{\pi j}). \tag{14}$$

They are separately defined for the π- and σ-polarization states and appropriately enumerated for the different scattering units by a subscript j

$$\begin{aligned}
\mathcal{A}_{\pi j} &= a_{\pi j} \exp(i\alpha_{\pi j}) = [\cos\varepsilon_\theta + \mathcal{F}_{\pi j}^{+1} i \sin\varepsilon_\theta] \exp(i\varepsilon_\pi), \\
\mathcal{B}_{\pi j} &= b_{\pi j} \exp(i\beta_{\pi j}) = [\cos\varepsilon_\theta + \mathcal{F}_{\pi j}^{-1} i \sin\varepsilon_\theta] \exp(i\varepsilon_\pi), \\
\mathcal{R}_{\pi j} &= r_{\pi j} \exp(i\rho_{\pi j}) = [\mathcal{F}_{\pi j}^{+1} \cos\varepsilon_\theta + i \sin\varepsilon_\theta] \exp(i\varepsilon_\pi), \\
\mathcal{S}_{\pi j} &= s_{\pi j} \exp(i\sigma_{\pi j}) = [\mathcal{F}_{\pi j}^{-1} \cos\varepsilon_\theta + i \sin\varepsilon_\theta] \exp(i\varepsilon_\pi).
\end{aligned} \tag{15}$$

The first two transmission factors define the step-like changes of the amplitude and phase of the same wave in the course of the scattering event. These factors can be used separately for each wave to determine local values of the refraction index and the extinction coefficient or both together to obtain a hyperbolic equation of the customary dynamic theory.

The last two reflection factors are ratios of the complex amplitudes of the transmitted waves to those incident ones and are, in general, different for the two polarization states. For the first and last dipole plane coinciding with external crystal boundaries they are identical with the global ones and define the crystal reflectivity for both polarization states.

The importance of the two local reflection factors as they are evaluated from a single plane view-point is to provide a formal tool enabling one to 'observe' an actual process of the wave field formation over the entire model cross-section from the lower to upper model external boundaries. It particularly refers to a real case situation where the second incident wave for the lower external surface in the model is absent. The local version of the reflection factors is essential for mapping the convergence process. This crucial process transforms the wave field from its casual version in the neighborhood of the lower crystal boundary into its *semi-periodic* or *periodic* versions in the neighborhood of its upper boundary. It can be, in a way, considered as the wave field convergence to its proper mode of interaction between the EM field and the radiating dipoles arranged in periodically spaced planes.

The convergence phenomenon in the wave field formation appears in the periodic or almost periodic structure models for some angular regions centered for each order of reflection around the Bragg angle. Its existence reflects a trend in the numerical solution obtained to approximate the proper state of the EM field-structure interaction for a particular incidence angle θ. This is valid only in the limit solution and can

be expressed in analytical terms and appropriately called *infinite* Bragg solution. It is equivalent to the solutions for so called 'symmetric Bragg case' resulting from the dynamic theory in the Darwin and Ewald-von Laue formulations.

The actual process of the wave field convergence can be best studied by help of the recurrence equation proposed below which relates the reflection factors derived for the two adjoining and identical units of scattering represented by a single dipole plane or by a set of such planes. From formula (12) we can write for each scattering unit the two following equations:

$$\begin{aligned} \mathbf{B}^{tr}_{\pi j} &= c_u \mathbf{A}^{in}_{\pi j+1} + d_u \mathbf{B}^{tr}_{\pi j+1}, \\ \mathbf{A}^{in}_{\pi j} &= a_u \mathbf{A}^{in}_{\pi j+1} + b_u \mathbf{B}^{tr}_{\pi j+1} \end{aligned} \tag{16}$$

which divided by sides yield the following recurrence formula as:

$$\mathcal{R}_{\pi j} = \frac{c_u + d_u \mathcal{R}_{\pi j+1}}{a_u + b_u \mathcal{R}_{\pi j+1}}, \quad \text{where } \mathcal{R}_{\pi j} = \frac{\mathbf{B}^{tr}_{\pi j}}{\mathbf{A}^{in}_{\pi j}} \text{ and } \mathcal{R}_{\pi j+1} = \frac{\mathbf{B}^{tr}_{\pi j+1}}{\mathbf{A}^{in}_{\pi j+1}}. \tag{17}$$

The recurrence formula just derived reveals an interesting mathematical feature of convergence, to some extent similar to that of the function cos. If the latter is consecutively applied over any argument from the open interval $(0,1)$ it results in the same convergence limit equal to the real number of .739085133215 given here with the twelve-digit precision. The recurrence formula if used the first time for the lowest dipole plane will result in a complex number of absolute value very close to zero. However, if repetitively applied a great number of times in an ascending dipole planes sequence will result in the limit in a double equality equation

$$\mathcal{R}_{\pi j} = \mathcal{R}_{\pi j+1} = \mathcal{R}_{\pi}. \tag{18}$$

The interval of wave field convergence coincides with the neighborhood of any angle θ which satisfies the Bragg equation. Its extension as well as the observed rate of convergence depends on many factors of a physical origin. The convergence limit is found by solving a quadratic equation resulting from (17 and 18) the actual solution of which will be postponed to the following section.

The wave field convergence gives origin to an idea of proper state of vibrations which is defined in a unique way for a given structure and for a defined incidence angle θ. We will denominate this state: *Geometric Fields Similarity* (GFS) since the equality (18) necessarily involves all others which relate the remaining factors:

$$\mathcal{F}_{\pi j} = \mathcal{F}_{\pi j+1} = \mathcal{F}_{\pi}, \quad \mathcal{A}_{\pi j} = \mathcal{A}_{\pi j+1} = \mathcal{A}_{\pi}, \quad \mathcal{B}_{\pi j} = \mathcal{B}_{\pi j+1} = \mathcal{B}_{\pi}. \tag{19}$$

It will be convenient to call all these factors, shown without the subscript j, *global* ones since they are valid for all the scattering units.

The GFS condition represents a kind of solution of the Maxwell equations for the periodic media which is characterized by a repetition of the amplitude ratios (factors) rather than the EM field itself and as such may be qualified as a *semi-periodic* solution. The resulting closed-form solution represents a proper state of vibration understood as a limiting case for the real case where the GFS condition cannot be satisfied, at least, for the last unit neighboring the lower boundary of a finite crystal.

In the latter case, as shown by the numerical tests exclusively, the EM field is being gradually built up from some irrelevant state of vibration at this unit to the values approximating each time closer the infinite Bragg solution while going up the consecutive scattering units as illustrated in Fig. 1. In consequence, the best approximation is reached at the very upper boundary of a thick perfect crystal.

The effect of the wave field convergence becomes even more rapid if the absorption takes up a significant value or if, for benefit of model testing, the value of charge density is artificially and drastically increased. In this situation the infinite Bragg solution is practically valid for all the units.

VII. INFINITE SOLUTION

The infinite Bragg solution is a direct result of the geometric fields similarity (GFS) which is satisfied for all the dipole planes in the model. In other words the local parameter $\mathcal{R}_{\pi j}$ becomes a global one valid for all the units and the crystal as a whole:

$$\mathcal{R}_{\pi j+1} = \mathcal{R}_{\pi j} = \mathcal{R}_{\pi j} = \mathcal{R}_{\pi B}, \tag{20}$$

where the subscript B indicates the Bragg crystal solution.

We recall again that the less stringent condition is used now for the required periodicity referred to the amplitude ratios than to the amplitudes, as is customary in the dynamic theory.

All the properties of proper state vibrations as defined by the GFS result from a simple formula to be given now. Joining the expressions (17) and (18) we get:

$$\mathcal{R}_{\pi j}/\mathcal{R}_{\pi j+1} = \mathbf{B}^{tr}_{\pi j}/\mathbf{A}^{in}_{\pi j} \cdot \mathbf{A}^{in}_{\pi j+1}/\mathbf{B}^{tr}_{\pi j+1} = 1 \tag{21}$$

and requiring continuity of the polarization vectors:

$$\begin{aligned} \mathbf{A}^{tr}_{\pi j} &= \mathbf{A}^{in}_{\pi j+1} = \mathbf{A}^{in}_{\pi j}\, \mathcal{A}_\pi \exp(-i\delta), \\ \mathbf{B}^{in}_{\pi j+1} &= \mathbf{B}^{tr}_{\pi j+1} = \mathbf{B}^{tr}_{\pi j}\, \mathcal{B}_\pi^{-1} \exp(\ \ i\delta) \end{aligned} \tag{22}$$

we finally obtain the looked for GFS condition:

$$\mathcal{A}_\pi\, \mathcal{B}_\pi = \exp(i2\delta) \quad \text{where} \quad \delta = k\, d_{hkl} \sin\theta \tag{23}$$

is the path phase angle δ, the same for all the scattering units.

From phase-relationship resulting from the GFS condition (23), while taking into account derived in paper II formulas for $\mathcal{A}_\pi$ and $\mathcal{B}_\pi$ (eq. 33) we immediately obtain the modified Bragg law:

$$2\,d_{hkl}\sin\theta = m\lambda\,(1+\frac{\alpha_\pi+\beta_\pi}{2\pi m}) \tag{24}$$

with α_π and β_π representing the phase shifts which both waves $A_{\pi j}^{in}$ and $B_{\pi j}^{in}$ suffer while being transmitted through each j-th scattering unit. The mean value of the both above phase shifts is responsible for the deviation of the modified Bragg law from its exact version.

From the amplitude relationship of the same basic GFS condition (23) we conclude that absolute values of both transmission factors $\mathcal{A}_\pi$ and $\mathcal{B}_\pi$ satisfy exactly the following equation of hyperbola:

$$a_\pi\, b_\pi = 1 \tag{25}$$

By joining the last result with that obtained in paper II (eqs. 34) for the relative phase shifts for $\varepsilon_{\alpha\pi}=\alpha_\pi-\varepsilon_\pi$ and $\varepsilon_{\beta\pi}=\beta_\pi-\varepsilon_\pi$ we get another dispersion-like equation correlating these phase shifts with the inter-wave phase angle φ_π and the structure-polarization sensitive angle ε_θ in a hyperbolic formula as:

$$\sin\varepsilon_{\alpha\pi}\,\sin\varepsilon_{\beta\pi} = \cos^2\varphi_\pi\,\sin^2\varepsilon_\theta \tag{26}$$

The equation obtained is an exact equivalent of the main equation of the Ewald-vonLaue dynamic theory where the inter-wave phase angle φ_π can assume values exactly equal to π for the first branch of the obtained hyperbola and 0 for the second one in a case of the odd valued reflection order m, and vice versa for the even valued of the latter.

In order to analyze a general relationship of inter-wave angle φ_π with all others angles appearing in (14) and (26) we again recall to the general GFS condition (23). Substituting there the expressions for both transmission factors $\mathcal{A}_\pi$ and $\mathcal{B}_\pi$, derived in paper II (eq. 31), we obtain the following identity:

$$\cos(2\varepsilon_\theta)+i\sin(2\varepsilon_\theta)\,\cosh(\Phi_\pi+i\varphi_\pi) = \exp[i2(\delta-\varepsilon_\pi)], \quad \text{where} \quad \Phi_\pi = \ln|\mathcal{F}_\pi|. \tag{27}$$

Since the absolute value of the left side of the above expression is equal unity we can obtain the following quadratic equation for the $\sinh\Phi_\pi$

$$\sinh^2\Phi_\pi - 2\cot(2\varepsilon_\theta)\sin\varphi_\pi\,\sinh\Phi_\pi - \sin^2\varphi_\pi = 0. \tag{28}$$

Solving it we get two formulas for the relationship between the inter-wave phase angle φ_π, the absolute value of the inter-wave factor $\mathcal{F}_\pi$ and the polarization-structure sensitive angle ε_θ which all are interrelated through the GFS condition. The two solutions are:

$$\sinh \Phi_\pi = \begin{bmatrix} I: -\sin\varphi_\pi \tan\varepsilon_\theta \\ II: \quad \sin\varphi_\pi \cot\varepsilon_\theta \end{bmatrix} = \frac{f_\pi - 1/f_\pi}{2}. \tag{29}$$

Substituting the solution I into (27) we get the following double equality:

$$y \equiv \frac{d-a}{2i\sqrt{bc}} = \cos\varphi_\pi \tag{30}$$

which enables one to evaluate the angle φ_π as a real number in terms of the introduced dimensionless parameter y if the absolute value of the latter is not greater than 1 or, in other words, if the angular region of the angle θ satisfies a set of inequalities:

$$|\sin(\delta - \varepsilon_\pi)| \leq |\sin\varepsilon_\theta| \quad \text{for} \quad |y| \leq 1. \tag{31}$$

Substituting the solution II into (27) we get the other double equality:

$$x \equiv \frac{a+d}{2} = \cos\varphi_\pi \tag{32}$$

which give means to evaluate the angle φ_π as a real number in terms of the second introduced parameter x if the absolute value of the latter is not greater than 1 or, in other words, if the angular region of the angle satisfies a second set of the inequalities:

$$|\cos(\delta - \varepsilon_\pi)| \leq |\cos\varepsilon_\theta| \quad \text{for} \quad |x| \leq 1. \tag{33}$$

The two solutions I and II for a given order of reflection m give rise to three diverse ranges for the angle θ separated by the two singular points. For the first of them, called the Laue point, the parameter $y = -1^m$ and the inter-waye phase angle $\varphi_\pi = \pi$. For the second one, termed the Ewald point, the parameter $y = -1^{m+1}$ and the respective inter-wave phase angle $\varphi_\pi = 0$. The above relations are valid for both states of polarization and corresponds to a situation in which the incident mesofield assumes the minimum and maximum values, respectively. These two points can be supplemented by a third singular one, conveniently called the Bragg point, for which the parameter y disappears and the inter-wave phase angle φ_π is exactly equal $\pi/2$. All these points for the whole range of the θ angles are shown in Fig. 2.

The Laue and Ewald points give rise to the three separate angular regions for the angle θ. Within each of them we define a real valued inter-wave phase angle φ and subsequently the factors $\mathcal{A}_\pi$, $\mathcal{B}_\pi$ and $\mathcal{R}_\pi$, which together with the $\mathcal{F}_\pi$-factor completely describe microscopic image of the EM field in all the scattering units of the model. We can trace factors such as $|\mathcal{R}_\pi|^2$ and $|\mathcal{T}_\pi|^2$ as a function of the angle θ at an arbitrary depth below the crystal surface in a form of calculated rocking curves (Fig. 1). One of these curves can be submitted to an experimental verification: absolute value of the $\mathcal{R}_\pi$-factor for the surface scattering unit.

The $\mathcal{R}_\pi$-factor is a function of path phase angle δ which, in turn, depends on the incidence angle θ. This function can be obtained by solving the following quadratic equation resulting from the recurrence formula (15) under the condition given by (16):

$$b_u\mathcal{R}_\pi^2 + (a_u - d_u)\mathcal{R}_\pi - c_u = 0 \tag{34}$$

The two solutions are given by:

$$\mathcal{R}_{\pi 1,2} = (y \pm \sqrt{y^2-1}) = \begin{bmatrix} \exp(i\cos^{-1} y) & for|y| \leq 1 \\ \exp(i\cosh^{-1} y) & for|y| > 1 \end{bmatrix} \tag{35}$$

where the parameter y can be defined in terms of the scattering matrix elements

$$y \equiv \frac{d_u - a_u}{2i\sqrt{b_u c_u}}. \tag{36}$$

The formulas (20-36) are given in terms of the angles ε_π and ε_θ for the π-polarization state. For the σ-state both above angles are substituted by the unique angle ε_σ.

We will introduce the second and complementary factor $\mathcal{T}_{\pi j}$ called a transmission parameter. It is defined as a ratio of the complex amplitudes of the incident beam transmitted through the $j+1$ unit to that transmitted through the unit j or:

$$\mathcal{T}_{\pi j} = \mathcal{A}^{in}_{\pi j+1}/\mathcal{A}^{in}_{\pi j} \tag{37}$$

From (14b) we obtain the relation between both parameters as

$$\mathcal{T}_{\pi j} = 1/(a_u + b_u\mathcal{R}_{\pi j+1}) \tag{38}$$

and the solution of the resulting from the GFS condition (23) another quadratic equation for $\mathcal{T}_\pi$

$$\mathcal{T}_{\pi 1,2} = (x \pm \sqrt{x^2-1}) = \begin{bmatrix} \exp(i\cos^{-1} x) & for|x| \leq 1 \\ \exp(i\cosh^{-1} x) & for|x| > 1 \end{bmatrix} \tag{39}$$

to define two values of the transmission factors $\mathcal{T}_{\pi 1}$ and $\mathcal{T}_{\pi 2}$ where a new parameter x was assumed to be

$$x \equiv \frac{a_u + d_u}{2}. \tag{40}$$

Both parameters introduced, y and x, are always real and for the primitive scattering unit satisfy an equation of ellipse with the half-axes $1/\sin\varepsilon_\theta$ and $1/cos\varepsilon_\theta$:

$$\sin^2\varepsilon_\theta\, y^2 + cos^2\varepsilon_\theta\, x^2 = 1 \tag{41}$$

where the Laue, Bragg and Ewald points for the first order of reflection are marked out on the ellipse by the coordinates $[-1,1]$, $[0,1/|\cos\varepsilon_\theta|]$ and $[1,-1]$ respectively.

Resuming, the Laue and Ewald points divide the entire region of the angles θ into two types: I for $|y| \leq 1$ and II for $|y| > 1$. The phase relationship between the two EM waves incident on each dipole plane, A_k^{in} and B_k^{in}, is defined by the real-valued inter-wave angle φ_π separately given for the two solution types I and II by the equations $\varphi_\pi = \arccos y$ and $\varphi_\pi = \arccos x$, respectively.

We identify the type I solution, extending between Laue and Ewald points with a center approximately at the Bragg point with a total reflection region TRR, since the absolute value of the $\mathcal{R}_B$-factor is constant and equal to unity. The positions of these three points, all fixed in the y-scale, if given in the θ-scale, depend on the two main factors, the superficial charge density and the state of polarization, in a quite different way.

The Laue point, for $y = -1$, which in the σ-state of polarization corresponds to the exact satisfaction of the unmodified Bragg law, is separated from the Ewald point by the angular θ distance roughly proportional to the value of charge density function. The distance between these two points in the σ-polarization state is reduced in size by a factor almost exactly equal to $\cos(2\theta)$ but is still centered about the Bragg point. The latter in both polarization states exactly satisfies equation: $\varphi = \pi/2$ where φ is defined before the inter-wave phase angle. The latter continuously changes from π to 0 when passing from the Laue to Ewald points while at the same time the absolute value of the R-factor is constant and equal to unity.

The primary extinction defined by the $\mathcal{F}_\pi$-factor with two exceptions for the Laue and Ewald points is always present and assumes it maximum value at the Bragg point. For the model of a single dipole planes it can be easily evaluated by the absolute value of the $\mathcal{F}_\pi$-factor equal to:

$$|\mathcal{F}_\pi| = (1 - \sin \varepsilon_\pi)/\cos \varepsilon_\pi \,. \tag{42}$$

In the II solution the absolute value of the $\mathcal{R}_\pi$-factor, no longer a constant, is rapidly declining in a manner predicted earlier by Darwin[1]. It has to be noted that it was not changed upon inclusion of the Ewald self-consistency principle, quite to the contrary of the conclusion arrived at by Zachariasen[20]. The latter acredited this difference between the respective curves derived from the Ewald theory to the lack of the self-consistency in the derivation of the Darwin formula for a single crystal plane.

The EM field composed of the two beams of equal absolute amplitudes is strictly periodic only for the two points, Laue and Ewald, which separate solutions obtained for the regions I and II. It is also periodic for all the points of the region corresponding to the type II solution but with the absolute amplitude values of the two beams different.

The Laue point for the σ-polarization state in the primitive scattering unit deserves a special attention. Its position evaluated in the θ scale corresponds to $y = -1^m$ where

the phase shift angles α and β are equal to 0 and the modified Bragg law, as shown by equation (24), is reduced to its exact version. The two incident waves reach the dipole plane with the same amplitude but with the opposite phase ($\varphi_\pi = \pi$). Since in this case there is no interaction whatsoever between the EM field and the dipoles of the scattering planes, these latter become for this field 'invisible'. Hence a conclusion to be drawn is that, at least, in the above model the exact Bragg law has a purely kinematic character.

VIII. REAL CASE MATRIX SOLUTION

We can treat now a particular but otherwise most important type of solution which almost exactly satisfies GFS pattern over the upper and main part of a big perfect crystal but which, at the same time, diverges from it substantially in the region neighboring its lower boundary. This situation results from absence in the real case of the second wave incident on the lowest dipole plane of a model, a fact which clearly breaks GFS pattern. The latter can only be restored in the upper region of a perfect crystal, if sufficiently thick, by an effect of the wave fields convergence. It is needless to say that this type of solution can only be studied by the numerical method and for this very reason it has been never approached.

A closed-form crystal solution valid for the above real case immediately results from the general solution (12), if we assume that all the dipole planes are identical. The corresponding matrix product (11) is obtained by help of the Chebyshev polynomials of the second kind taking into account that the scattering unit matrix $\mathbf{M}_u$ is unimodular and that its elements on both diagonals are in complex conjugate relation with both properties now being extended for the matrix product $\mathbf{M}_c$ and its matrix elements as shown below

$$\begin{bmatrix} \mathbf{A}_{11}^{in} \\ \mathbf{B}_{11}^{tr} \end{bmatrix} = \mathbf{M}^c \begin{bmatrix} \mathbf{A}_{KJ}^{tr} \\ 0 \end{bmatrix} \quad \text{where} \tag{43}$$

$$\mathbf{M}_c = \mathbf{M}_u^N = \begin{bmatrix} a_u U_{n-1}(x) - U_{n-2}(x) & b_u U_{n-1}(x) \\ c_u U_{n-1}(x) & d_u U_{n-1}(x) - U_{n-2}(x) \end{bmatrix} . \tag{44}$$

The matrix elements a_u, b_u, c_u and d_u are given by (6), the variable x is defined by (39) and the Chebyshev polynomials of the second kind are of a standard type:

$$U_{n-1}(x) = \frac{\sin(N \arcsin\sqrt{1-x^2})}{\sqrt{1-x^2}} . \tag{45}$$

The global value $\mathcal{R}_\pi$ determined from (35) becomes a parameter valid for the whole crystal model $\mathcal{R}_\pi^c$ and is obtained from the equation:

$$\mathcal{R}_\pi^c = \frac{\mathbf{B}_{\pi 1}^{tr}}{\mathbf{A}_{\pi 1}^{in}} = \frac{c_u U_{n-1}(x)}{a_u U_{n-1}(x) - U_{n-2}(x)} . \tag{46}$$

This equation enables one to calculate the reflecting power for a crystal of finite and arbitrary thickness as a square of the absolute value of $\mathcal{R}_\pi^c$.

The conservation of energy for the whole model is easily verified if we calculate a crystal transmission factor defined from:

$$\mathcal{T}_\pi^c = \frac{\mathbf{A}_{\pi n}^{tr}}{\mathbf{A}_{\pi 1}^{in}} = \frac{1}{a_u U_{n-1}(x) - U_{n-2}(x)} . \tag{47}$$

Both transmission and reflection factors satisfy conservation energy identity:

$$|\mathcal{R}_\pi^c|^2 + |\mathcal{T}_\pi^c|^2 = \frac{b_u c_u U_{n-1}^2(x) + 1}{a_u d_u U_{n-1}^2(x) - 2x U_{n-1}(x) U_{n-2}(x) + U_{n-2}^2(x)} = 1 . \tag{48}$$

The above matrix formulation of the scattering problem takes into account the multiple scattering effects not only within the individual dipole planes but also between the different dipole planes of the same model. The matrix method initiated by the pioneering analysis of Abeles[15] is fully described in the Born and Wolf[16] classical monograph. The main difference is contained here in a definition of the matrix elements. These latter, correctly defined by both the Hertz vector formalism and the Ewald self-consistency satisfy energy conservation of the system, regarded without absorption. Conservation of energy in this case, given as the sum of amplitudes squared of the two incident and two transmitted waves, refers equally to 'macroscopic' or global as well as to 'microscopic' or local scattering problems.

The matrix method is particularly convenient for verifying the convergence of the EM wave fields from the general to Bragg (GFS) solution in a hybrid connection of both solutions required for the real case situation. Since both above solutions are of a microscopic type, the approach developed enables one to identify all the components of the stationary EM field formed by the two interacting waves at any point within the crystal space. It is also possible to calculate any chosen scattering parameter as a function of the angle θ in the form of appropriate diffraction profiles ('rocking' curves) for planes situated at different levels of 'depth' inside the crystal and within a full range (0-90 deg) of the angle θ making thus the analyzed convergence phenomenon quite transparent. A gradual build up of the EM field, from that given by the general (kinematic) solution, characterized by the zero amplitude value of the reflected wave at the lower crystal boundary, to the Bragg (dynamic) solution at its surface was shown in Fig. 1. For benefit of model testing, a similar EM field build up from the kinematic to dynamic diffraction profile while drastically increasing the charge density value, from the usually found value to some extremal one is illustrated in Fig. 3 for the (111)-Ge reflection and in Fig. 4 for the two reflections (620)-Si, bordering the angle $\theta = \pi/2$ on both sides.

IX. CONCLUSIONS

The fact that the basic dynamic X-ray diffraction theories have been developed in terms of differential equations rather than in terms of the Fourier integrals used in the kinematic theory[24] may find in this bridging type of approach a new interpretation resulting from its two main attributes:

- The plane waves summation is carried out inside the crystal space rather than in infinity as in the Fourier transform theory.
- It enables one to take into account the self-consistent dipoles interaction to the overall scattering pattern making the intuitive Darwin approach fully comparable with the treatments of Ewald and Laue.

If the latter is insignificant the results obtained would coincide with those obtained by Fourier integrals. This interaction, formalized by Ewald's self-consistency principle, increases with number of dipoles in the correct crystal sites and contributes in the form of non-linear terms to the overall diffraction pattern. These terms becomes predominant in a saturation stage leading to effects such as the total reflection range. This emerged saturation stage, a typically non-linear phenomenon, makes the Fourier integral approach in describing diffraction phenomena quite inadequate. On the other hand, the analytical-numerical procedure developed may be considered as an extension of the Fourier transform into the non-linear yet energy-conservation area of applications.

The differences and similarities with the conventional dynamic theories can be resumed in some points of importance:

- While the formalism developed makes use of the most important self-consistency principle due to Ewald in all the scattering models with full rigor it follows rather the ideas of Planck and Lorentz who let the single dipole be excited by an electrical force, which consists of two parts, the 'external' one and a second contribution which comes from the other dipoles of the body.
- The present model is able to match continuously those features of X-ray scattering on crystals which are separately treated by either kinematic or dynamic theories; the aspect to be applied in the heterolayers scattering.
- In this model the charge density value can be arbitrarily increased without any effect of Darwin's 'excess' scattering[1].
- Since the EM field attains the best convergence to its proper state of vibrations at the very crystal surface, the perfection state of the latter becomes quite irrelevant[25,26].
- Only the unit concept can make the matrix method for exact solution of the Darwin difference equation really effective[11,14].

- The dispersion-like hyperbola curve obtained in this approach has only illustrative value. However, a comparison with its current usage may be of interest:

  - The dispersion-like hyperbola is derived in an exclusively analytical way in contrast to the usual geometric arguments resulting from so-called boundary conditions. In consequence, it is exact and suffers no restrictions (e.g. the complex angle θ) if it is used in the vicinity of $\theta = \pi/2$ region.
  - In contrast to conventional dynamic theories we don't have to introduce the index of refraction as an external parameter. In fact, it is intrinsically built into the self-consistent approach. It can assume its proper values for each order of reflection; it depends on the magnitude of absolute amplitude of each of the two interacting waves and automatically follows all the changes in superficial charge density if applied to scattering problems in heterostructures.
  - The hyperbola equation appears in the coordinate frame other than the Fourier space.

Our last remark to be made here is that the present results, obtained without any intermediary approximations and using the correct model of the radiation, may represent the first step of a more fundamental approach to the problem of dynamic, self-consistent X-ray scattering for more than two interacting beams.

X. ACKNOWLEDGMENTS

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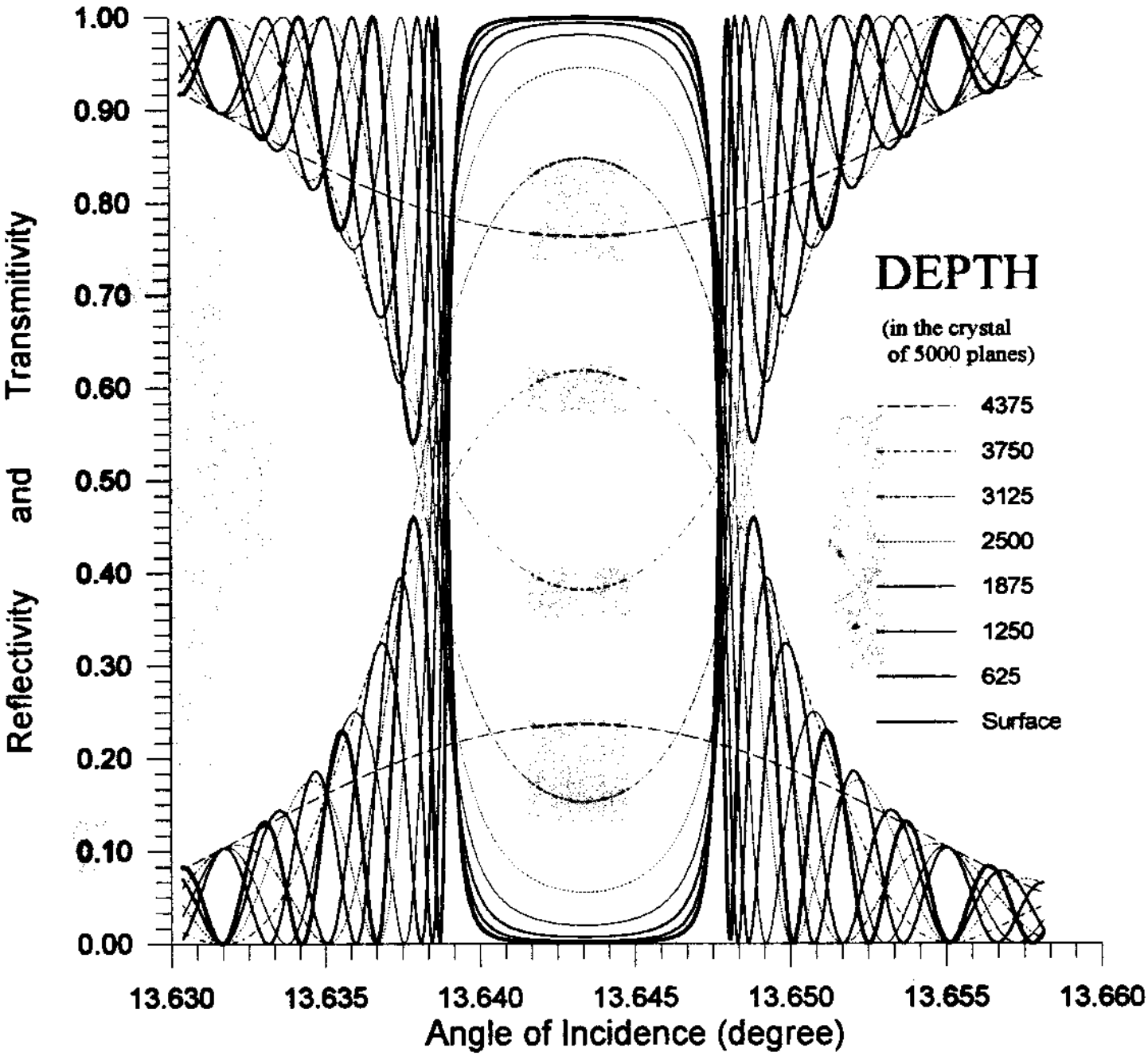


Fig. 1

FIG. 1. Dependence of reflectivity and transmitivity for both waves on depth inside the crystal for (111)-Ge reflection and radiation wavelength $CuK_{\alpha 1}$.

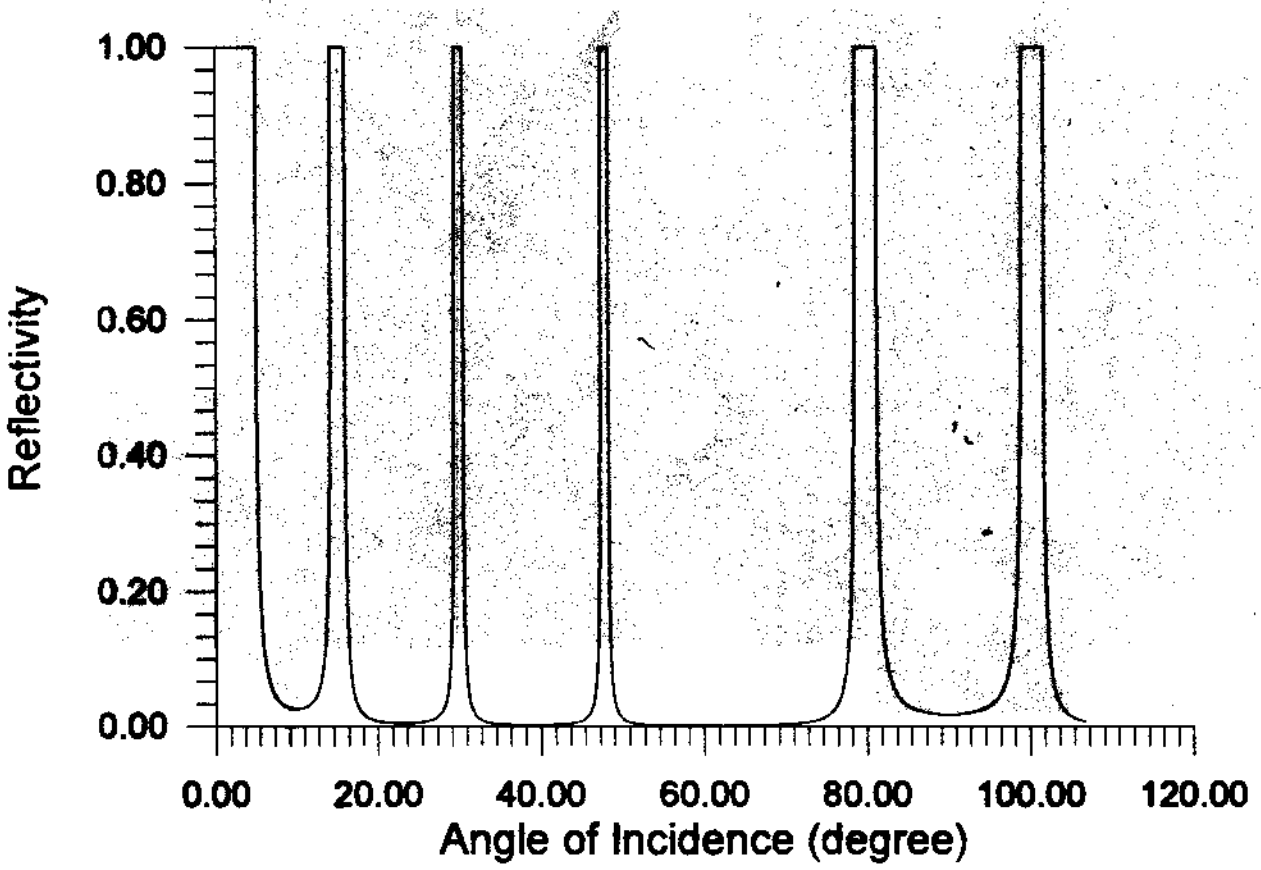
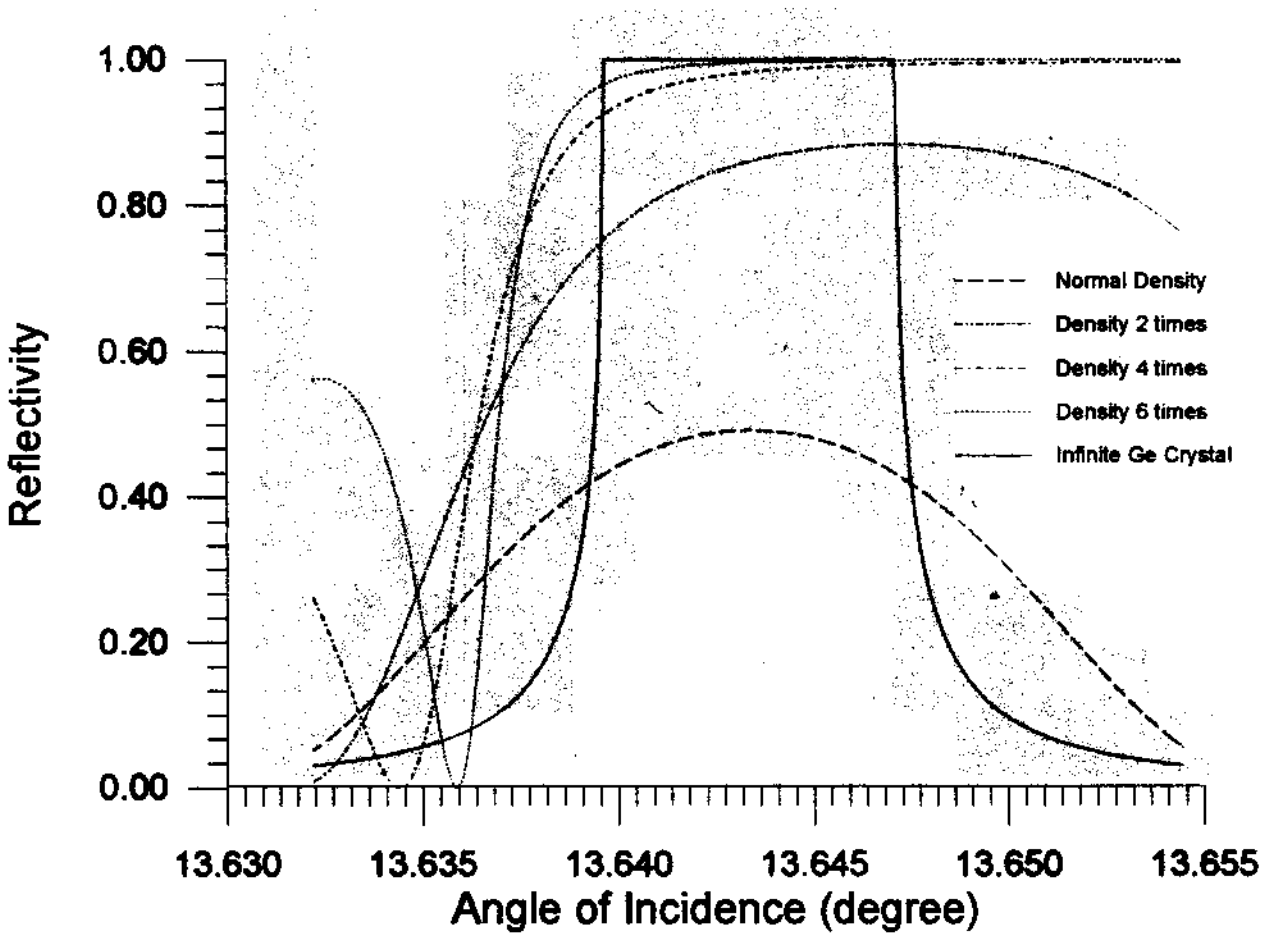


Fig. 2

FIG. 2. Dependence of reflectivity on diffraction angle θ within interval [0,110] degree under increased charge density value by factor 10^3.



Reflectivity with the different planar charge density
for 1024 dipoles planes versus Ge infinite crystal

Fig. 3

FIG. 3. Continuous transformation of the diffraction profile from kinematic to dynamic type as a function of charge density value for (111)-Ge reflection and radiation wavelength $CuK_{\alpha 1}$.

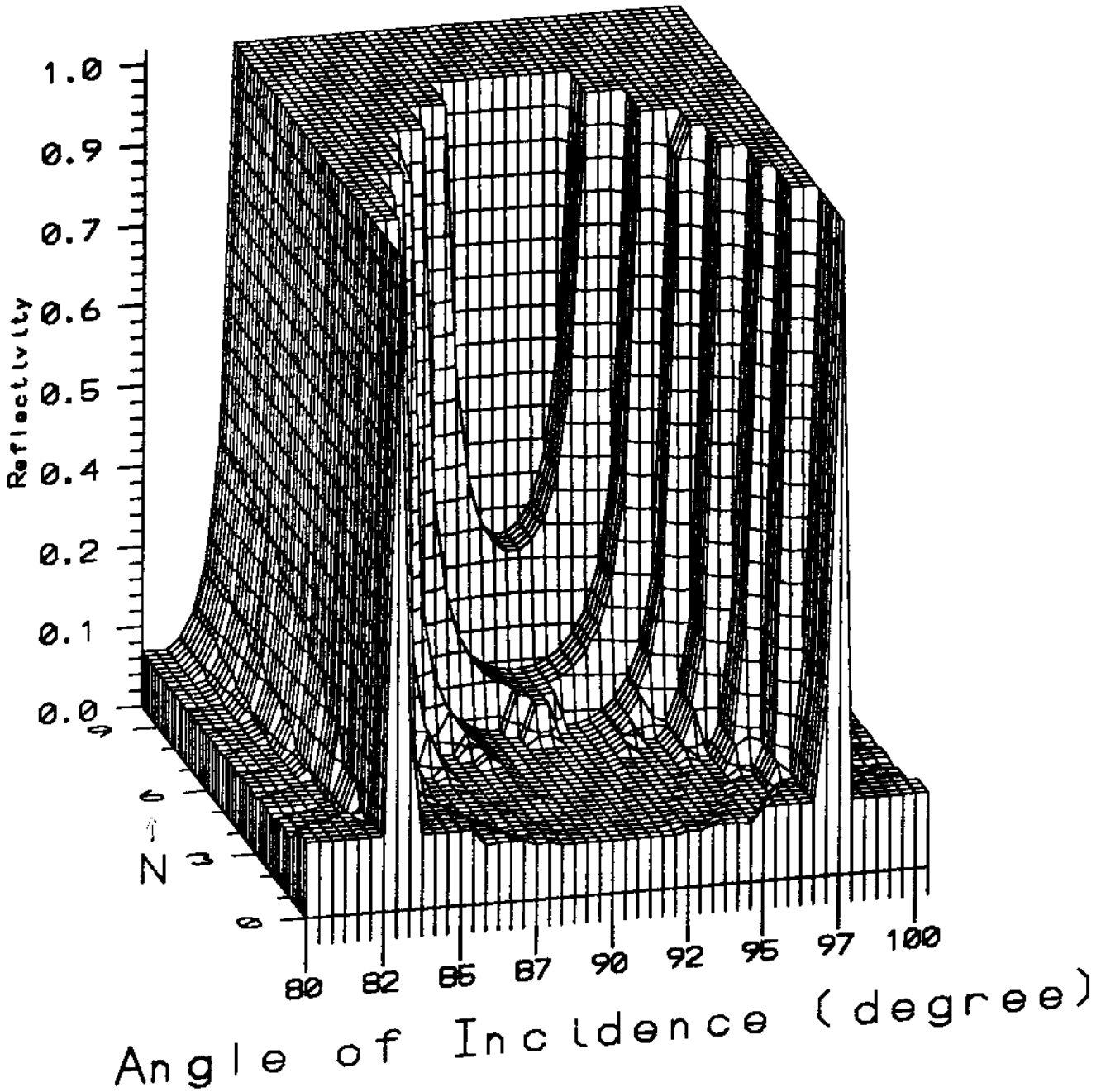


FIG. 4. Continuous transformation of the diffraction profile from kinematic to dynamic type as a function of charge density value ($\sigma = \sigma_0 \times 2^N$) for the two (620)-Si reflections, bordering the angle $\theta = \pi/2$. Assumed radiation wavelength $1.23456.10^{-10}m$.

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