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X-UV synthetic interference mirrors : theoretical approachB. Pardo ⁽¹⁾, T. Megademini ⁽¹⁾ and J. M. André ⁽²⁾⁽¹⁾ Institut d'Optique, UA 14 CNRS, Bât. 503, 91405 Orsay Cedex, France⁽²⁾ Laboratoire de Chimie Physique, UA 176 CNRS, 11 rue P. et M. Curie, 75231 Paris, Cedex 05, France*(Reçu le 25 juillet 1987, révisé le 9 juin 1988, accepté le 24 juin 1988)*

Résumé. — Cet article a pour objectif de donner les éléments théoriques nécessaires pour le calcul et l'optimisation des miroirs interférentiels dans le domaine du rayonnement X-UV. Il présente une revue des méthodes existantes ainsi qu'un ensemble de résultats originaux. L'utilisation de la méthode de Hill pour la résolution de l'équation de propagation dans un milieu périodiquement stratifié conduit à une nouvelle formulation des conditions de Bragg. Une large place est consacrée à la méthode matricielle qui introduit naturellement des invariants de grande importance. Les principales méthodes récurrentes de calcul de la réflectivité sont brièvement exposées. Le problème des imperfections est envisagé. Afin de prendre en compte les erreurs d'épaisseur, les univers statistiques qui en permettent l'étude cohérente sont définis. Le formalisme matriciel est utilisé pour traiter de l'influence de la rugosité interfaciale à l'aide du modèle de la couche homogène de transition. Enfin, en concurrence avec les cavités résonnantes Fabry-Pérot, l'utilisation de structures périodiquement stratifiées comme amplificateur est proposée.

Abstract. — The purpose of the paper is to give the theoretical basis for the design and optimization of X-UV interference mirrors. To achieve this original results are presented and the « state of the art » methods are reviewed. A new formulation of the Bragg conditions is obtained on the basis of the « Hill method » to solve the wave propagation equation in a periodically stratified medium. A large part of the paper is devoted to matricial formalism. The major role played by invariant quantities is emphasized. Recursive procedures to compute the reflectance are summarized. The problems of imperfections are also considered. Concerning the thickness errors, statistical universes are defined to give a coherent treatment of their effects. The matricial formalism is adopted to treat the influence of the interfacial roughness using the homogeneous transition layer model. Finally the perspective of a distributed X-UV amplifier in a periodic multilayered structure is proposed as an alternative to the Fabry-Perot resonator.

Introduction.

Synthetic mirrors designed for the X-UV radiation consist in a periodic stack of bilayers whose thickness is of the same order of magnitude as the wavelength, typically from a few tenths of nm to a few hundred of nm. In fact these reflectors constitute bandpass interference filters whose resonance condition is non other than the well-known Bragg law.

The theoretical study of such structures is needed for two main reasons :

- to predict and optimize the optical performance of projected devices ;
- to determine the characteristics of multilayered structures realized for optical or others (metallurgical) purposes.

Roughly speaking, there are two main theoretical approaches to calculate the optical properties (reflectance, bandpass...) of these X-UV structures. They originate from studies carried out in very different spectral regions : the visible (optical) spectrum and the X-ray region.

In the framework of the optical approach, the systematic study of the stratified media, whose a pile of films is a particular case, has been achieved by Abelès [1]. His work initially dealt only with transparent materials, but can easily be extended to the X-UV domain where the photoabsorption is large, by substituting a complex index to the real refractive and by considering the tangential component of the complex wavevector instead of the refractive angle.

As far back as 1931, Kiessig [2] used an optical

approach to explain the interference fringes observed with X-ray radiation incidents on grazing incidence a thin film coating a substrate. Parratt [3] in 1954 again adopted an optical method to account for the effects of contaminant layers on the X-ray specular reflection. Studies concerning the X-ray grazing reflection from thin films have been extensively carried out, in particular by Croce *et al.* They observed in the early seventies the influence of the surface irregularities and of the thickness dispersion on the interference fringe contrast [4]. This group made a pioneering use of computers both for the control of a high precision X-ray goniometer and for theoretical simulations. A large amount of software has been developed and in particular the so-called impedance method for the calculation of the reflectance of a multilayered structure. With the advent of X-UV interference mirrors the optical methods have been largely extended to the X-ray regime either with the matricial formalism [5-7] or with recursive procedures [8, 9] to predict the optical performances (reflectance, bandwidth, spectral response...).

On the other hand the methods developed by Darwin, Prins, Laue and Ewald to interpret the diffraction diagrams in X-ray crystallography can be applied to the periodic multilayered structures. Their theories constitute for the essential the so-called dynamical theory [10]. In 1977, Vinogradov and Zeldovich have presented on the basis of the dynamical theory, the general principles and the possibilities of X-UV mirrors for normal incidence [11].

The dynamical theory calls upon (at least implicitly) the Floquet theorem [12] which constitutes the basis of the mathematical development of the theories dealing with phenomena occurring in periodic structures. Among such phenomena, the propagation of nearly free electrons in crystals initially studied by Bloch [13] and Brillouin [14] who introduced the concept of forbidden band, should be mentioned. The analogy between the optics of periodic stratified media and the electron band theory (E.B.T.) in crystalline solids is very close ; for instance we show that the concept of forbidden gaps in the E.B.T. is associated to the Bragg reflection of the X-ray radiation in periodic multilayered mirrors. The Floquet theorem concerns the linear differential equations of the second order with periodic coefficients with the Hill equation [15] appearing in the study of the Lunar motion as a well-known particular case. We show that the method developed by Hill to solve this equation enables us to find a close and compact relation describing the propagation of an electromagnetic wave in a periodic stratified medium and leading to a generalization of the Bragg conditions.

In the spectral domain of interest, it can be expected that the various inhomogeneities affect the

optical performances more considerably as in visible spectrum. Among the imperfection, the interfacial roughness has given rise to extensive studies. The pioneer work of Croce *et al.* [4] and the more recent papers of Rosenbluth and Forsyth [16], Vidal and Vincent [17], Megademini and Pardo [18] should be mentioned. The other kind of important imperfection is the so-called thickness errors. This problem has been little studied in comparison with the roughness effects. The notable contributions are limited to the studies of Rosenbluth, Forsyth and Spiller [16, 19].

The paper is organized as follows :

the first section deals with the stratified medium optics where the Abelès works play a major role. The case of the periodic medium is treated in its generality using the « Hill method ». The second section develops the matricial formalism and the case of the bilayered structure is treated in detail. The third part is devoted to the recursive procedures of computation borrowed from the optical spectrum and extended to the X-UV regime. The following section gives a critical discussion of the macroscopic approach adopted in the previous parts. Finally we discuss the imperfection effects, mainly the thickness errors and the influence of interfacial roughness.

1. Stratified medium optics.

1.1 STRATIFICATION. — A stratified medium is a structure whose properties depend only upon one coordinate. We limit the study to the Cartesian coordinates. The study for the curvilinear ones would be of considerable interest for the design of optical devices such as telescopes or reflection microscopes. To our knowledge little work has been devoted to the curvilinear problem. This is not surprising considering the complexity of the Cartesian case. For this purpose, one could advantageously use the approaches adopted to treat the X-ray diffraction by bent crystals [20]. In fact the Cartesian results can be extended to curved optical tools without the risk of large errors provided the radius of curvature is big with respect to the wavelength.

The assumption of a plane stratification offers two important possibilities :

— the transverse electric waves and the transverse magnetic waves can be distinguished. The former denoted by T.E. or S are linearly polarized waves with the electric field parallel to the planes of stratification. The latter denoted by T.M. or P, are also linearly polarized waves but with the magnetic field parallel to the stratification. This distinction is not restrictive since an arbitrarily wave can be decomposed into two linearly polarized waves, one of which is a T.E. wave and the other a T.M. wave ;

— the Snell-Descartes law is fulfilled. From an

elementary point of view this law stipulates that the product $n \cdot \sin(r)$ where n and r stand respectively for the real refractive index and the refractive angle, is an invariant quantity. Actually it expresses the conservation of the tangential component of the wavevector. The law results from the plane stratification. In the case of a spherical stratification the momentum of the wavevector $n \cdot R \cdot \sin(r)$ where R is the radius will be conserved.

In the X-UV region, the absorption is not negligible, contrary of visible optics. Absorption is taken into account by using a complex index \tilde{n} and consequently the refraction angle becomes complex. It is convenient to decompose the wavevector \mathbf{k} into an invariant tangential component \mathbf{k}_\parallel and a perpendicular component \mathbf{k}_\perp which can be deduced from the tangential one by setting the square k^2 proportionnal to the square of refractive index \tilde{n} . The Snell-Descartes law is then written

$$k_\parallel^2 + k_\perp^2 = \tilde{n}^2 k_0^2 \tag{1}$$

with k_0 the wavenumber in vacuum, given by $2\pi/\lambda$ or ω/c , where λ is the wavelength in vacuum, ω the angular frequency of the radiation and c the light velocity in vacuum. On the other hand, the medium is non magnetic so that the magnetic permability is set to be equal to unity. The angle i is the angle of incidence. Traditionally in the X-UV domain, the glancing angle $\theta = \frac{\pi}{2} - i$ is used rather than i .

1.2 THE ABELÈS EQUATIONS. — In its generality, the problem consists in solving the Maxwell equations. When we want to explicit these relations, we face the choice of the system of units. In optics, the Gauss system is probably the simpler one since it explicit the velocity of the light c and displays the symmetry between the electric \mathbf{E} and magnetic \mathbf{H} fields

$$\text{curl } \mathbf{E} = -\frac{1}{c} \frac{\partial}{\partial t} \mathbf{H} \tag{2a}$$

$$\text{curl } \mathbf{H} = \frac{\tilde{n}^2}{c} \frac{\partial}{\partial t} \mathbf{E} . \tag{2b}$$

Abelès has treated the problem in a nearly exhaustive way [1]. We introduce the components E_x, E_y, E_z of the electric field and H_x, H_y, H_z of the magnetic field in a reference system shown in figure 1 ; the z -axis is the direction of stratification. The radiation travels in the y - z plane and the incident beam propagates in the positive z direction. The x, y axis are parallel to the planes of stratification. The Abelès method consists in writing the components so that the Snell-Descartes law is taken into account explicitly. The relevant boundary

conditions are then automatically satisfied for any glancing angle. It yields :

$$\begin{aligned} E_x &= U(z) \exp(i \cdot k_\parallel \cdot y) \exp(-i \cdot \omega \cdot t) \\ E_y &= 0 \\ E_z &= 0 \end{aligned} \tag{3}$$

T.E. wave

$$\begin{aligned} H_x &= 0 \\ H_y &= V(z) \exp(i \cdot k_\parallel \cdot y) \exp(-i \cdot \omega \cdot t) \\ H_z &= W(z) \exp(i \cdot k_\parallel \cdot y) \exp(-i \cdot \omega \cdot t) \end{aligned}$$

$$\begin{aligned} H_x &= U(z) \exp(i \cdot k_\parallel \cdot y) \exp(-i \cdot \omega \cdot t) \\ H_y &= 0 \\ H_z &= 0 \end{aligned}$$

T.M. wave \tag{4}

$$\begin{aligned} E_x &= 0 \\ E_y &= -V(z) \exp(i \cdot k_\parallel \cdot y) \exp(-i \cdot \omega \cdot t) \\ E_z &= -W(z) \exp(i \cdot k_\parallel \cdot y) \exp(-i \cdot \omega \cdot t) \end{aligned}$$

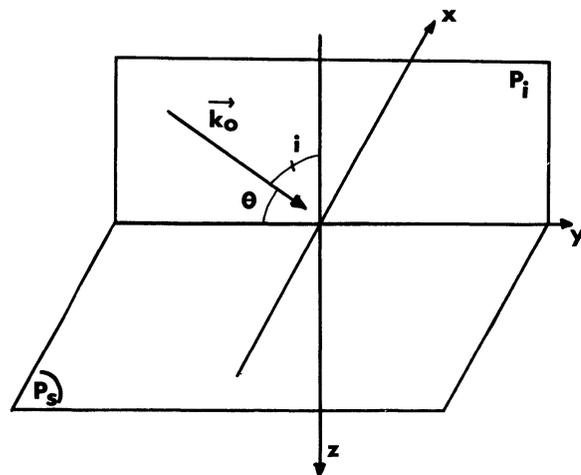


Fig. 1. — Cartesian reference system ; P_i plane of incidence, P_s plane of stratification.

In the following, the time-dependent term and the tangential term will be omitted for simplicity. The amplitudes $U(z)$ et $W(z)$ are connected by the Maxwell equations :

$$W = -U \cos(\theta) \quad \text{T.E. wave} \tag{5}$$

$$W = -\frac{U}{\tilde{n}^2} \cos(\theta) \quad \text{T.M. wave} . \tag{6}$$

Similarly, $U(z), V(z)$ and $U'(z), V'(z)$ (the prime denoting differentiation with respect to z) are related through a system of two linear

differential equations of the first order, which can be written in a matricial form as follows :

$$\begin{pmatrix} U' \\ V' \end{pmatrix} = ik_0 \begin{pmatrix} 0 & 1 \\ \frac{k_{\perp}^2}{k_0^2} & 0 \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} \quad \text{T.E. wave} \quad (7a)$$

$$\begin{pmatrix} U' \\ V' \end{pmatrix} = ik_0 \begin{pmatrix} 0 & \tilde{n}^2 \\ \frac{1}{\tilde{n}^2} \frac{k_{\perp}^2}{k_0^2} & 0 \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} \quad \text{T.M. wave} \quad (7b)$$

To solve the system of coupled equations (7), V can be eliminated to obtain a linear differential equation of the second order :

$$U'' + k_{\perp}^2(z) \cdot U = 0 \quad \text{T.E. wave} \quad (8a)$$

and

$$U'' - \frac{d(\ln(\tilde{n}^2))}{dz} U' + k_{\perp}^2(z) \cdot U = 0 \quad \text{T.M. wave} \quad (8b)$$

If we set : $U = F \cdot \tilde{n}$ in equation (8b), the equation for the T.M. wave can be rewritten in terms of F'' and F in a form similar to equation (8a) for the T.E. wave :

$$F'' + h^2(z) F = 0 \quad (8c)$$

with

$$h^2(z) = k_{\perp}^2(z) - \frac{d^2 \ln(\tilde{n})}{dz^2} - \left(\frac{d \ln(\tilde{n})}{dz} \right)^2 \quad (8d)$$

In the following of the section, we restrict the problem to the T.E. wave, since the study can be extended to the T.M. waves in a straightforward manner by substituting $h(z)$ to $k(z)$.

For our study, it is interesting to discuss equation (8a) in the three following cases.

1.2.1 The medium is homogeneous. — The equation (8a) is reduced to the simple form

$$U'' + k_{\perp}^2 \cdot U = 0 \quad (9)$$

where k_{\perp} does not depend upon the variable z . The well-known general solution is given by :

$$U(z) = \frac{A^+}{\sqrt{k_{\perp}}} \exp(ik_{\perp} \cdot z) + \frac{A^-}{\sqrt{k_{\perp}}} \exp(-ik_{\perp} \cdot z) \quad (10)$$

where k_{\perp} is introduced for comparison with the next case. The expression (10) shows that the field can be decomposed into two plane waves, travelling in opposite directions along the z -axis. It is worth to note that the two waves are independent and the

existence of one of them does not infer the existence of the other.

1.2.2 The medium is slightly inhomogeneous. — Equation (8a) can be treated in the framework of the geometrical optics according to which, the solution are quasi-plane waves propagating along the light path.

The complete solutions take the approximate form :

$$U(z) = \frac{A^+}{\sqrt{k_{\perp}(z)}} \exp\left(i \int^z k_{\perp}(z) dz\right) + \frac{A^-}{\sqrt{k_{\perp}(z)}} \exp\left(-i \int^z k_{\perp}(z) dz\right) \quad (11)$$

The results obtained for the homogeneous case are preserved for the main points. The field is still decomposed into two quasiplane waves, but their amplitudes vary slightly as a function of the index, via $k_{\perp}(z)$.

The relation (11) is analogous to the result obtained from the B-K-W (Brillouin-Kramers-Wentzel) method developed for quantum mechanic problems [21].

1.2.3 The medium is periodically stratified. — This case is fundamental for our study, since the X-UV interference mirrors usually realized have a periodic structure. This situation is discussed in the next section.

1.3 PERIODICALLY STRATIFIED MEDIUM. — The period of the structure is denoted by d . The coefficients k^2 (and h^2) in equations (8a) and (8b) are periodic with period d . According to the Floquet theorem [12] the complete solution has the general form :

$$U(z) = A_1(z) \exp(iK_1 \cdot z) + A_2(z) \exp(iK_2 \cdot z) \quad (12)$$

where $A_1(z)$ and $A_2(z)$ are periodic with period d . The field is still decomposed into two quasiplane waves whose variable amplitudes reflect the periodicity of the structure. The crux of the problem is to determine the Bloch-Floquet wavenumbers K_1 and K_2 . Once this is done, the determination of A_1 and A_2 presents comparatively little difficulty. To solve this question, the method developed by Hill for the study of the Lunar motion can be applied [15]. It appears [22] that K_1 and K_2 are the opposite roots of the following equation :

$$\sin^2 \left(K \frac{d}{2} \right) = \Delta(0) \sin^2 \left(k_0 \sqrt{J_0} \frac{d}{2} \right) \quad (13a)$$

where J_0 is the constant term in the Fourier expansion $J(z)$ of k^2/k_0^2 . Let us note that J_0 has the same expression for the T.E. and the T.M. waves ;

$\Delta(K)$ is an infinite determinant whose elements depend upon the components J_p of $J(z)$, the vacuum wavenumber k_0 and the reciprocal constant $g = 2 \cdot \pi / d$

$$\Delta(K) = \begin{vmatrix} 1 & \frac{J_{-1} k_0^2}{k_0^2 J_0 - (K - g)^2} & \frac{J_{-2} k_0^2}{k_0^2 J_0 - (K - g)^2} & \frac{J_{-3} k_0^2}{k_0^2 J_0 - (K - g)^2} & \dots & \dots \\ \frac{J_1 k_0^2}{k_0^2 J_0 - K^2} & 1 & \frac{J_{-1} k_0^2}{k_0^2 J_0 - K^2} & \frac{J_{-2} k_0^2}{k_0^2 J_0 - K^2} & \dots & \dots \\ \frac{J_2 k_0^2}{k_0^2 J_0 - (K + g)^2} & \frac{J_1 k_0^2}{k_0^2 J_0 - (K + g)^2} & 1 & \frac{J_{-1} k_0^2}{k_0^2 J_0 - (K + g)^2} & \dots & \dots \\ \dots & \dots & \dots & 1 & \dots & \dots \\ \dots & \frac{J_q k_0^2}{k_0^2 J_0 - (K + qg)^2} & \dots & \dots & \dots & \dots \end{vmatrix} \quad (13b)$$

The convergence of this kind of infinite determinant was studied by Poincaré [23].

Relation (13a) is of fundamental importance for the study of the propagation in the periodically stratified media. We limit our discussion to the case where the absorption can be neglected. Different situations occur, taking into account that $\Delta(0)$ is real :

i) $J_0 > 0, \Delta(0) > 0$ and

$$\Delta(0) \cdot \sin^2 \left(k_0 \sqrt{J_0} \frac{d}{2} \right) < 1 :$$

in these conditions the wavenumber K is real. The two waves propagate in the structure without attenuation ;

ii) $J_0 < 0$: the « averaged » refractive index $1 - \delta$ (δ is assumed to be positive) is less than unity and the glancing angle is smaller than the corresponding critical angle, so that total reflection takes place. In the latter case, the wavenumber K is imaginary. There are two other cases where K is also complex :

a) $J_0 > 0, \Delta(0) > 0$ but

$$\Delta(0) \cdot \sin^2 \left(k_0 \sqrt{J_0} \frac{d}{2} \right) > 1 : \quad (14a)$$

b)

$$J_0 > 0, \Delta(0) < 0. \quad (14b)$$

The two waves can only travel parallel to the direction of stratification ; one of them is evanescent and the other is not excited since its amplitude would increase exponentially with z . The regimes a) and b) correspond to Bragg reflection.

The system of inequalities (14a) and (14b) constitutes the Bragg conditions. This leads to a generalization of the usual Bragg law

$$2 d \sin (\theta) = p \lambda \quad (15)$$

where p is the order of reflection, which is simply

obtained with kinematic theory by writing that the difference of optical path between two rays reflected by two consecutive interfaces is an integral multiple of λ .

If we set $K = \text{Re} (K) + i \text{Im} (K)$, the conditions :

— (14a) is satisfied when

$$\text{Re} (K) = (2l + 1) \cdot \frac{\pi}{d} \quad (l \text{ integer}) \quad (16a)$$

and $\text{Im} (K) \neq 0$, so that

$$\sin^2 \left(K \cdot \frac{d}{2} \right) = \text{ch}^2 \left(\text{Im} (K) \cdot \frac{d}{2} \right) > 1 \quad (16b)$$

— (14b) is satisfied when

$$\text{Re} (K) = 2 \cdot l \cdot \frac{\pi}{d} \quad (l \text{ integer}) \quad (17a)$$

and $\text{Im} (K) \neq 0$, so that :

$$\sin^2 \left(K \cdot \frac{d}{2} \right) = -\text{sh}^2 \left(\text{Im} (K) \cdot \frac{d}{2} \right) < 0. \quad (17b)$$

A necessary condition for Bragg reflection is according to relations (16a) and (17a) :

$$\text{Re} (K) = \frac{p \cdot g}{2}. \quad (18)$$

Condition (14a) corresponds to odd order Bragg reflections for which $\sin^2 (k_0 \sqrt{J_0} d/2) \cong 1$ and (14b) corresponds to even order Bragg reflection for which $\sin^2 (k_0 \sqrt{J_0} d/2) \cong 0$.

Consequently

$$k_0 \sqrt{J_0} \frac{d}{2} \cong p \cdot \frac{\pi}{2} \quad (19a)$$

that is,

$$2 \sqrt{J_0} d \cong p \cdot \lambda. \quad (19b)$$

For a periodic bilayered structure consisting of material 1 (refractive index $n_1 = 1 - \delta_1$, thickness d_1) and material 2 (refractive index $n_2 = 1 - \delta_2$, thickness $d_2 = (1 - \gamma) d$), relation (19b) gives by expliciting J_0 , the usual Bragg law which takes into account the refraction effect, in terms of the vacuum wavelength λ and the glancing angle θ :

$$2 \cdot d \cdot \sin(\theta) \cdot \left(1 - \frac{\bar{\delta}}{\sin^2(\theta)}\right) = p \cdot \lambda, \quad (20a)$$

$$\bar{\delta} = \gamma \cdot \delta_1 + (1 - \gamma) \cdot \delta_2. \quad (20b)$$

For a given wavelength λ the Bragg condition (18) is satisfied within a domain $\Delta\theta$ of glancing angle centered at the value given by relation (19), value usually called Bragg angle. Reciprocally, this angular domain defines a range Δk_0 for the vacuum wavenumber k_0 where the Bragg reflection can take place. In the particular but usual case of a bilayered structure, a rather tedious algebra gives an approximate expression of Δk_0 , for first Bragg order reflection :

$$\frac{\Delta k_0}{k_0} = \frac{8}{\pi^2} \sqrt{\frac{2}{3}} |\delta_1 - \delta_2| \frac{\sin(\gamma\pi)}{\sin^2(\theta)}. \quad (21)$$

The above discussion can be summarized with the help of a diagram (Fig. 2). This diagram is analogous to the band schemes encountered in the electronic

band theory (E.B.T.) of crystals. The wavenumber is plotted along the ordinate, and the real part $\text{Re}(K)$ of the Bloch wavenumber K is stated along the abscissa. The discontinuities for k_0 appear for the values $p \cdot g/2$ of $\text{Re}(K)$ which correspond to the limits of the Brillouin zones in the E.B.T. By analogy with the E.B.T., the relation

$$\left. \frac{\partial k_0}{\partial \text{Re}(K)} \right|_{pg/2} = 0 \quad (22)$$

is expected. Following this analogy, one can say that the forbidden bands in the E.B.T. are equivalent in the optics of periodically stratified media to domains of k_0 where the propagation of waves along the z -direction is forbidden (evanescent waves) for the bilayered structure. Let us note that the widths of the gaps Δk_0 can be more directly obtained in the framework of the matricial formalism.

2. Matricial formalism.

The matricial formalism can be introduced naturally owing to the linear character of the system of Abelès equations (7). It can be shown that, if the value of (U, V) is known at z_0 then the value of (U, V) at z can be obtained by a matricial relation

$$\begin{pmatrix} U \\ V \end{pmatrix}_z = \hat{g}(z, z_0) \begin{pmatrix} U \\ V \end{pmatrix}_{z_0}. \quad (23)$$

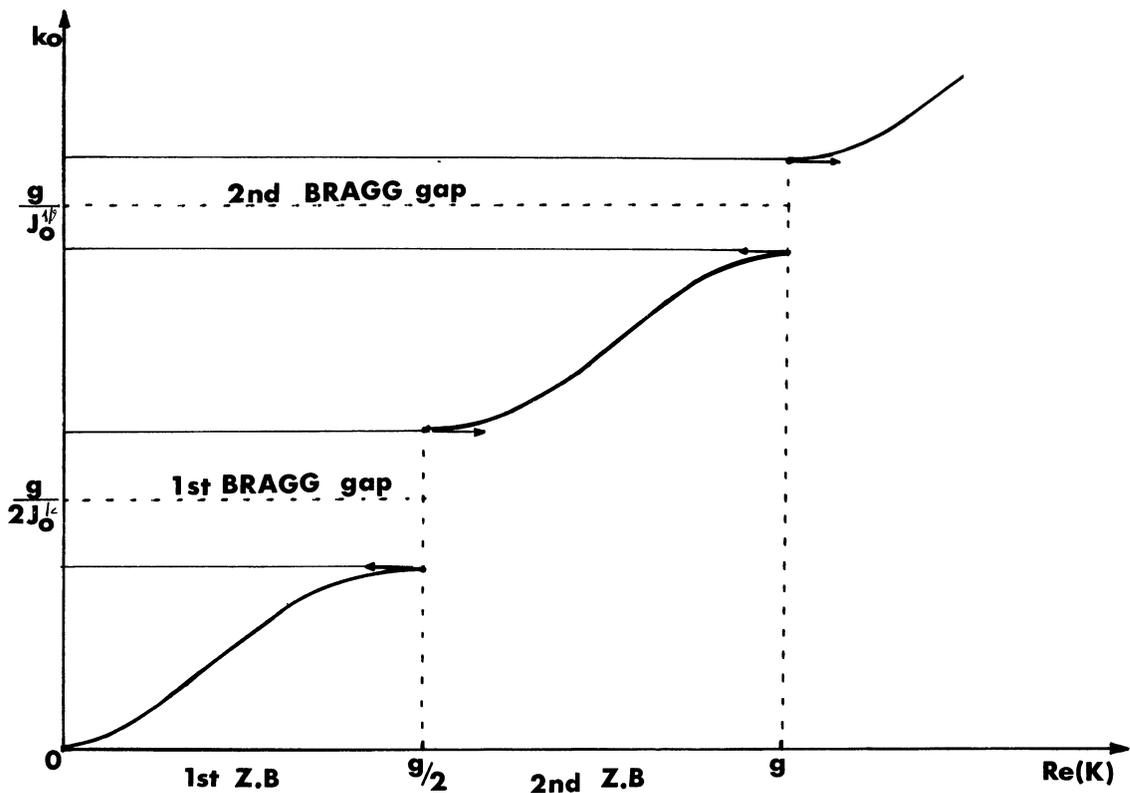


Fig. 2. — Dispersion curve in the k_0 - $\text{Re}(K)$ plane ; Z.B. denotes the Brillouin zone.

The operator $\hat{g}(z, z_0)$ is the characteristic propagator of the medium contained between the two planes situated at z_0, z respectively. By using relation (23) in the differential system (7) and taking account the following relation :

$$\hat{g}(z, z_0) = \hat{g}(z) \cdot \hat{g}^{-1}(z_0) \tag{24}$$

it results that $\hat{g}(z, z_0)$ satisfies the same differential equation as (U, V)

$$\frac{d}{dz} \cdot \hat{g}(z, z_0) = D(z) \cdot \hat{g}(z, z_0) \tag{25}$$

where $D(z)$ stands for the matrix appearing in equation (7a) or (7b) according to the polarization. This transformation has led from a system of two differential equations to a system of four differential equations which is not *a priori* a simplification. Nevertheless in the case of a stack of homogeneous layers $D(z)$ is constant inside each layer. It becomes formally :

$$\hat{g} = \exp(D \cdot z) \tag{26}$$

where

$$\exp(D \cdot z) = \sum_{n=0}^{\infty} \frac{D^n}{n!} z^n. \tag{27a}$$

A simple algebra gives :

$$\hat{g}(z) = \begin{pmatrix} \cos(k_{\perp} \cdot z) & \frac{i}{\xi} \sin(k_{\perp} \cdot z) \\ i \cdot \xi \cdot \sin(k_{\perp} \cdot z) & \cos(k_{\perp} \cdot z) \end{pmatrix} \tag{27b}$$

with

$$\xi^2 = \tilde{n}^2 - \cos^2(\theta) = \frac{k_{\perp}^2}{k_0^2} \quad \text{T.E. waves} \tag{28a}$$

and

$$\xi^2 = \frac{\tilde{n}^2 - \cos^2(\theta)}{\tilde{n}^4} = \frac{k_{\perp}^2}{\tilde{n}^4 k_0^2} \quad \text{T.M. waves} . \tag{28b}$$

The matrix is unitary, i.e. the determinant equals unity. In relation (28), the parameters are complex except for the glancing angle.

Until now, the Abelès formalism has been used. It amounts to study the tangential components of the electric and magnetic fields.

A more pedestrian approach used by several authors [5, 18] consists in decomposing the field into two plane waves that must satisfy the Snell-Descartes law, one of them T propagating in the positive z -direction and the other R in the opposite direction.

$$\begin{aligned} T &= A^+ \exp(i \cdot k_{\perp} z) \\ R &= A^- \exp(-i \cdot k_{\perp} z) \end{aligned} \tag{29}$$

A^{\pm} represents the electric field in the case of T.E. waves or the magnetic field in the case of T.M. waves.

Let us emphasize that the two representations are obviously equivalent. The (U, V) representation offers the advantage of taking into account directly the continuity relations, but when one has to compute the reflectance or the transmittance the passage to the (T, R) representation is forced finally. On the other hand the (T, R) representation is well suited to the study of roughness effects (see sect. 5). It is evident that in the new representation (T, R) the propagator $\hat{G}(z)$ has the simple diagonal form

$$\hat{G}(z) = \begin{pmatrix} \exp(i \cdot k_{\perp} \cdot z) & 0 \\ 0 & \exp(-i \cdot k_{\perp} \cdot z) \end{pmatrix}. \tag{30}$$

The matrix which allows (T, R) to be expressed in terms of (U, V) is a similarity matrix that transforms the propagator \hat{g} in Abelès representation into its diagonal form in the new representation. The problem then leads to a diagonalization of \hat{g} . From relation (30) it follows that the two eigenvalues Λ^{\mp} are the inverse of each other (\hat{g} is unitary) and are obviously given by :

$$\Lambda^{\mp} = \exp(\mp i \cdot k_{\perp} z). \tag{31}$$

Two eigenvectors e^{\mp} belonging to Λ^{\mp} respectively are :

$$e^{\mp} = \begin{pmatrix} 1 \\ \mp \xi \end{pmatrix}. \tag{32}$$

The transformation matrix and its inverse are given in terms of the elements of e^{\mp} :

$$P = \begin{pmatrix} 1 & 1 \\ \xi & -\xi \end{pmatrix} \tag{33a}$$

$$P^{-1} = \frac{1}{2} \begin{pmatrix} 1 & \frac{1}{\xi} \\ 1 & -\frac{1}{\xi} \end{pmatrix}. \tag{33b}$$

We note that P transforms (T, R) into (U, V) while P^{-1} gives, of course, the inverse transformation. These relations enable us to find directly the so-called Fresnel matrix F which gives the transformation of the (T, R) fields at the crossing through the surface separating two media 1, 2 (see Fig. 3) :

$$\begin{pmatrix} T \\ R \end{pmatrix}_2 = F \begin{pmatrix} T \\ R \end{pmatrix}_1. \tag{34a}$$

It is sufficient to perform the following procedure :

- passage from the (T, R) to the (U, V) representation in the medium 1, using the P_1 matrix ;
- passage through the 1, 2 boundary with the (U, V) representation by the identity matrix, since (U, V) are continuous ;

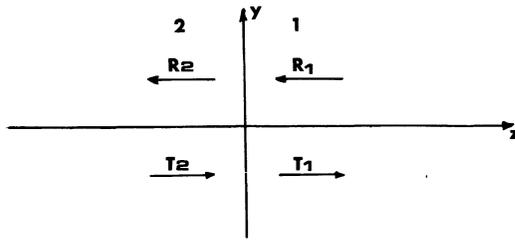


Fig. 3. — Bilayer system for the calculation of the Fresnel matrix in the (T, R) representation.

— passage from the (U, V) to the (T, R) representation in medium 2, using the P_2^{-1} matrix. It follows that the Fresnel matrix F in the (T, R) representation is

$$F = P_2^{-1} \cdot P_1 \tag{34b}$$

that is :

$$F = \frac{1}{2} \begin{pmatrix} 1 + \frac{\xi_1}{\xi_2} & 1 - \frac{\xi_1}{\xi_2} \\ 1 - \frac{\xi_1}{\xi_2} & 1 + \frac{\xi_1}{\xi_2} \end{pmatrix} \tag{34c}$$

The matrix F leads to the well-known Fresnel relations by setting conditions such that in the medium 1 there is only a transmitted wave. The reflection amplitude coefficient $r_{2,1}$ and the transmission amplitude coefficient $t_{2,1}$ are respectively :

$$r_{2,1} = \frac{R_2}{T_2} = \frac{\xi_2 - \xi_1}{\xi_2 + \xi_1} \tag{35a}$$

$$t_{2,1} = \frac{T_1}{T_2} = \frac{2 \xi_2}{\xi_1 + \xi_2} \tag{35b}$$

The matrix F can be rewritten using the Fresnel coefficients $r_{2,1}, t_{2,1}$:

$$F = \frac{1}{t_{2,1}} \begin{pmatrix} 1 & r_{2,1} \\ r_{2,1} & 1 \end{pmatrix} \tag{36}$$

It is worth noting that while $r_{2,1}$ and $t_{2,1}$ do not verify the relation :

$$|r_{2,1}|^2 + |t_{2,1}|^2 = 1 \tag{37}$$

but the useful relation

$$r_{2,1}^2 + t_{1,2} t_{2,1} = 1 \tag{38}$$

is true.

The relation (37) is often confused with the energy conservation law expressed in terms of reflectance \mathcal{R} and transmittance \mathcal{T} :

$$\mathcal{R} + \mathcal{T} = 1 \tag{39}$$

For each representation, the determination of the propagators and of the transfer matrices at a boundary (Fresnel matrix) enables us to solve completely the problem of the wave propagation in a pile of parallel films that presents no imperfection (roughness, bulk inhomogeneity).

PERIODIC STACK OF HOMOGENOUS BILAYERS. —

The stack consists of two alternating homogenous materials, denoted respectively by 1 and 2, characterized by their complex refractive index \tilde{n}_1 and \tilde{n}_2 and their thicknesses d_1 and d_2 . The Snell-Descartes law leads to the normal components $k_{1\perp}$ and $k_{2\perp}$ of the wavenumber k . N is the number of bilayers. The characteristic matrix of the whole medium is equal to the N -th power of the characteristic matrix M_{bi} of a bilayer :

$$M = (M_{bi})^N \tag{40}$$

In the (U, V) representation, M_{bi} is given by :

$$M_{bi} = \begin{pmatrix} \cos(k_{\perp 2} d_2) & \frac{i}{\xi_2} \sin(k_{\perp 2} d_2) \\ i \xi_2 \sin(k_{\perp 2} d_2) & \cos(k_{\perp 2} d_2) \end{pmatrix} \begin{pmatrix} \cos(k_{\perp 1} d_1) & \frac{i}{\xi_1} \sin(k_{\perp 1} d_1) \\ i \xi_1 \sin(k_{\perp 1} d_1) & \cos(k_{\perp 1} d_1) \end{pmatrix} \tag{41}$$

In the (T, R) representation the product is easy to performed and M_{bi} is given by :

$$M_{bi} = \frac{1}{1 - r^2} \begin{pmatrix} \exp(i\Phi) - r^2 \exp(-i\Delta) & r(\exp(-i\Phi) - \exp(i\Delta)) \\ r(\exp(i\Phi) - \exp(-i\Delta)) & \exp(-i\Phi) - r^2 \exp(i\Delta) \end{pmatrix} \tag{42a}$$

with

$$\Phi = \Phi_1 + \Phi_2 \quad \Delta = \Phi_1 - \Phi_2 \tag{42b}$$

where

$$\Phi_i = k_{\perp i} d_i \quad \text{and} \quad r^2 = r_{1,2}^2 \tag{42c}$$

To write M with the help of the elements C_{ij} of the matrix M_{bi} , we implement the method developed by Abelès [24] which used the Chebyshev Polynomials of the second kind $U_n(x)$ [25]

$$U_n(x) = \frac{\sin [(n + 1) x]}{\sin (x)} . \tag{43}$$

It gives (See appendix B)

$$M = \begin{pmatrix} C_{11} U_{N-1}(Kd) - U_{N-2}(Kd) & C_{12} U_{N-1}(Kd) \\ C_{21} U_{N-1}(Kd) & C_{22} U_{N-1}(Kd) - U_{N-2}(Kd) \end{pmatrix} \tag{44}$$

where the argument of the Chebyshev Polynomials has been written in the form $K \cdot d$ (d is the period, $d = d_1 + d_2$) to introduce the Bloch-Floquet wavenumber previously met in the general theory (see Sect. 1.2). It is expressed with the help of the trace S of the bilayer matrix M_{bi} , which has the same value in the two representations. Indeed a trace is an invariant of a matrix which undergoes a similarity transformation.

We get :

$$Kd = \cos^{-1} \left(\frac{S}{2} \right) . \tag{45a}$$

From relation (42) it results that :

$$S = \frac{2}{1 - r^2} [\cos (\Phi) - r^2 \cos (\Delta)] . \tag{45b}$$

The relation (45b) can be rewritten in a form similar to (13) :

$$\sin^2 \left(\frac{Kd}{2} \right) = \frac{1}{1 - r^2} \sin^2 \left(k_0 J^+ \frac{d}{2} \right) - \frac{r^2}{1 - r^2} \sin^2 \left(k_0 J^- \frac{d}{2} \right) \tag{46a}$$

$$J^+ = \frac{\tilde{n}_2 \sin (\theta_2) d_2 + \tilde{n}_1 \sin (\theta_1) d_1}{d} \tag{46b}$$

with

$$J^- = \frac{\tilde{n}_2 \sin (\theta_2) d_2 - \tilde{n}_1 \sin (\theta_1) d_1}{d} . \tag{46c}$$

A discussion based on relations (46) could be developed in a same way as in section 1.2. The main interest of this reformulation of the dispersion relation is to easily provide the widths of the forbidden bands (i.e., Bragg peaks).

In the no absorption case it turns out (see appendix A) that the Bragg gapwidths are given in terms of wavenumber in vacuum k_0 and glancing angle by :

$$\Delta k_0 = \frac{4}{d \cdot \sin (\theta)} |r \cdot \sin (p \cdot \gamma \cdot \pi)| . \tag{47}$$

The relation (47) is of a great interest, because it provides important information for the design of mirrors. First it appears that larger is the coefficient

of reflection of the bilayer, broader is the Bragg bandwidth. Moreover selection rules can be deduced. When γ is rational ; $\gamma = m/q$ where m and q are whole numbers whose HCF is one ($q > m$), the p -th Bragg gap is cancelled provided that the order p is a multiple of q . For instance, the condition $\gamma = 1/2$ is sufficient to reject all the even-order Bragg reflections. In this case, the odd-order Bragg gapwidths get their maximum value :

$$\Delta k_0 = \frac{4 \cdot r}{d \cdot \sin (\theta)} . \tag{48}$$

A very attractive property of the X-UV synthetic interference mirrors is the ability to choose freely the values of γ and as a consequence to reject some Bragg harmonics. This property is used to account for the design of premonochromator [26]. Another interesting property of these devices is offered by the possibility to fixe the period d and therefore to control the Bragg angle. Polarizing effects can then be achieved since the reflectance vanishes for the T.M. waves when the incident angle reaches the Brewster angle [27].

Reflectance and transmittance :

The reflectance \mathcal{R} and the transmittance \mathcal{T} of the periodic bilayered structure can be obtained in a close form, by assuming there is no R wave in the emerging medium (substrate). Then

$$\mathcal{R} = \rho \rho^* \tag{49}$$

$$\text{with } \rho = \frac{C_{21} U_{N-1}(Kd)}{C_{11} U_{N-1}(Kd) - U_{N-2}(Kd)}$$

$$\mathcal{T} = \tau \cdot \tau^* \tag{50}$$

$$\text{with } \tau = (C_{11} U_{N-1}(Kd) - U_{N-2}(Kd))^{-1} .$$

The latter expressions are strictly valid only when the extreme media are composed with the same material as the multilayered structure (i.e., medium 1 or 2). In practice they can be applied without large systematic errors when the real part of the refractive index is close to unity, the glancing angle much large than the critical angles and the number of bilayer N

sufficiently large. These conditions are generally satisfied for the X-UV interference mirrors.

When N becomes very large, the reflectance \mathcal{R} tends towards a limit \mathcal{R}_∞ . \mathcal{R}_∞ could be computed from (49), but it is more convenient to use directly the eigenelements of the matrix M_{bi} :

$$\begin{pmatrix} T \\ R \end{pmatrix}_1 = [M_{bi}]^N (a^+ \mathbf{Z}_+ + a^- \mathbf{Z}_-) \quad (51)$$

then

$$\begin{pmatrix} T \\ R \end{pmatrix}_1 = a^+ P_+^N \mathbf{Z}_+ + a^- P_-^N \mathbf{Z}_- \quad (52)$$

where P_+ , P_- and $\mathbf{Z}_+ = \begin{pmatrix} V_+ \\ W_+ \end{pmatrix}$, $\mathbf{Z}_- = \begin{pmatrix} V_- \\ W_- \end{pmatrix}$ are respectively the eigenvalues and the associated eigenvectors of M_{bi} (see appendix B). The subscript 1 refers to the incident medium (vacuum).

Since the modulus of P_- is less than unity:

$$\lim_{N \rightarrow \infty} \begin{pmatrix} T \\ R \end{pmatrix}_1 = a^+ P_+^N \begin{pmatrix} V_+ \\ W_+ \end{pmatrix} \quad (53)$$

and whence

$$\rho_\infty = \frac{R_\infty}{T_\infty} = \frac{W_+}{V_+}. \quad (54)$$

When the number of bilayers increases, the reflectance \mathcal{R} tends towards \mathcal{R}_∞ with possibly attenuated oscillations depending upon the strength of the absorption. See figure 4. These oscillations disappear

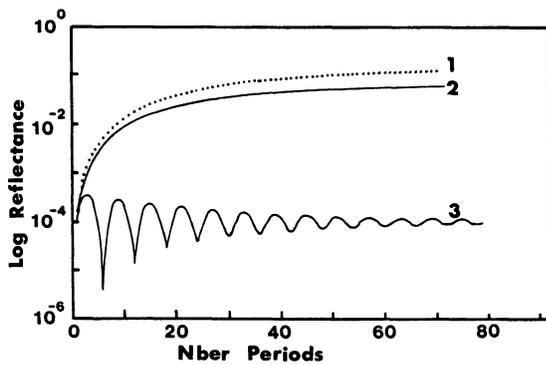


Fig. 4. — Reflectivity versus number of periods for different γ ratios: 1) order $p = 1$, $\gamma = 1/2$; 2) $p = 1$, $\gamma = 1/3$; 3) $p = 5/3$, $\gamma = 1/3$.

when the Bragg conditions are fulfilled. \mathcal{R} depends on the relative thickness of each layer, that is on γ . The problem of the optimization of γ to make \mathcal{R}_∞ maximum, is then met for practical purposes. As shown in appendix B, ρ_∞ can be written as:

$$\rho_\infty = \exp(i \Phi_2) [A + \sqrt{A^2 - 1}] \quad (55a)$$

with

$$A = \frac{\sin(\Phi)}{2 \cdot r \cdot \sin(\Phi_1)}. \quad (55b)$$

A condition to ensure the optimization is:

$$\frac{d\rho_\infty}{d\Phi_1} \approx \frac{dA}{d\Phi_1} = 0 \quad (56)$$

where $\varphi_1 = \text{Re}(\Phi_1)$.

When the Bragg law is satisfied, A varies with φ_1 as:

$$\frac{(\beta_1 - \beta_2) \varphi_1 + \beta_2 \pi}{\sin(\varphi_1)} \quad (\text{where } \beta \text{ is the imaginary part of the index}).$$

Then the condition $dA/d\varphi_1 = 0$ leads to the Vinogradov-Zeldovich relation (11):

$$\tan(\varphi_1) = \varphi_1 - \frac{\beta_2}{\beta_2 - \beta_1} \pi. \quad (57)$$

3. Recursive computation procedures.

Throughout this section, the notations will refer to figure 5 which gives the schematic representation of a multilayered structure, which is not necessary strictly periodic. We present two methods to calculate the reflectance of such structures, which are well suited to the use of a computer since the involved procedure is recursive.

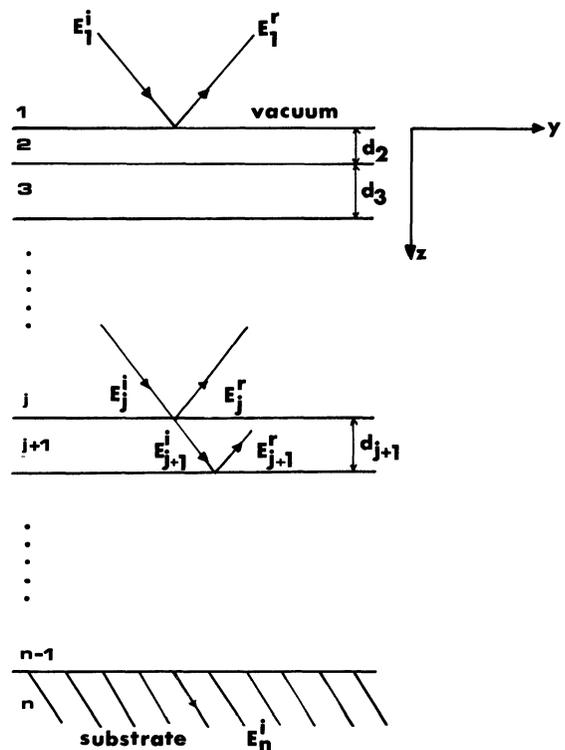


Fig. 5. — Multilayered system used for the recursive computation procedures: Parratt method, impedance method.

3.1 PARRATT METHOD. — This procedure is a generalization of the method initially developed by Parratt to account for the effects of contaminating layers in X-ray grazing specular reflection [3]. The initial approach has been modified to be valid at any glancing angle and extended to the T.M. waves. The continuity relations of the tangential components of the electric and magnetic fields provide a recursion relation for $\rho_{j-1,j}$

$$\rho_{j-1,j} = a_{j-1}^4 \left[\frac{\rho_{j,j+1} + r_{j-1,j}}{1 + \rho_{j,j+1} r_{j-1,j}} \right] \quad (58a)$$

where
$$\rho_{j-1,j} = a_{j-1} \left(\frac{E_{j-1}^r}{E_{j-1}^i} \right) \quad (58b)$$

E_{j-1}^i being the amplitude of the electric field of the wave incident on the boundary between the $j - 1$ -th and the j -th layers, and E_{j-1}^r the amplitude of the electric field reflected from this interface. For the two cases of polarization $r_{j-1,j}$ is the Fresnel coefficient of reflection given by the relation (35a) and a_j is the amplitude factor for half of the thickness d_j :

$$a_j = \exp \left(i \cdot k_{\perp j} \cdot \frac{d_j}{2} \right) \quad (59)$$

The computational procedure starts at the bottom of the stack, by setting $\rho_{n-1,n} = 0$ and works backward to the first medium where $a_1 = 1$, to give finally $\rho_{1,2}$ and the reflectance $\mathcal{R} = \rho_{1,2} \cdot \rho_{1,2}^*$.

The method borrowed from the optics of the visible spectrum has been widely used by several authors to predict the performance of X-UV multilayered structures [8, 9]. For the sake of illustration, the reflectance of a Fabry-Perot etalon

versus the glancing angle, at the Cu-L wavelength is plotted in figure 6.

3.2 IMPEDANCE (ADMITTANCE) METHOD. — The characteristic quantity is then the so-called impedance Z (admittance Y) that is the ratio of the tangential component of the electric field E to the tangential component of the magnetic field H (ratio of the magnetic component to the electric one) :

$$Z = \frac{E}{H} \quad \text{and} \quad Y = \frac{H}{E}. \quad (60)$$

The impedance is used for the case of the T.M. waves and the admittance for the T.E. waves. As the principle is the same in both cases of polarization, we restrict our attention to the T.M. case.

The impedance Z_j in the j -th the layer at the j -th boundary between the j -th and $(j - 1)$ -th layer is :

$$Z_j = \frac{E_j^i + E_j^r}{H_j^i + H_j^r}. \quad (61)$$

We define the iterative impedance z and the coefficient of reflection α respectively by :

$$z = \frac{E^i}{H^i} = \frac{E^r}{H^r} \quad (62)$$

$$\alpha = - \frac{E^r}{E^i} = \frac{H^r}{H^i}. \quad (63)$$

The iterative impedance is invariant within a homogeneous medium and is given by :

$$z = \frac{k_{\perp}}{\tilde{n}^2} \quad (64)$$

in the polarization case considered.

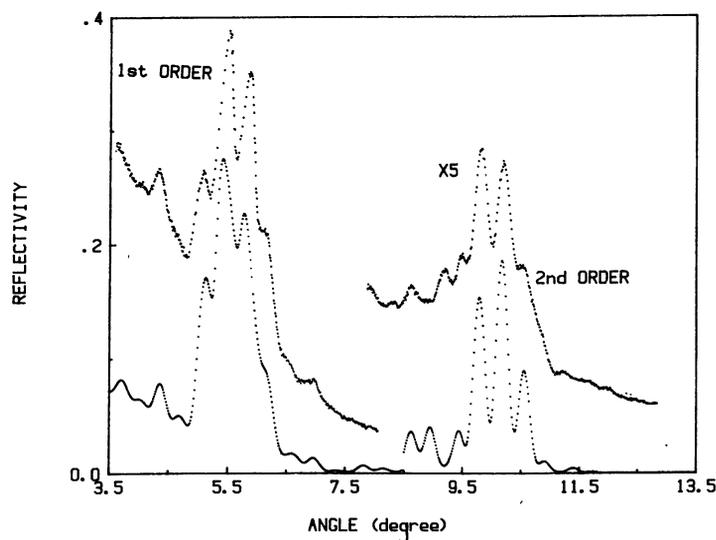


Fig. 6. — Reflectivity *versus* glancing angle of a Fabry-Perot etalon computed by the Parratt method (bottom curves) in comparison with experimental data (top curves) at $\lambda = 1.33$ nm (Cu-L emission) for the first and second order (from Ref. [28]).

From (61), (62) and (63), it follows that :

$$Z_j = z_j \frac{1 - \alpha_j}{1 + \alpha_j}. \quad (65)$$

The coefficient α'_{j-1} at the same j -th boundary is given in terms of the impedance Z'_j in the $j - 1$ -th layer at the same $(j + 1)$ -th boundary

$$\alpha'_{j-1} = \frac{z'_{j-1} - Z'_j}{z'_{j-1} + Z'_j}. \quad (66)$$

The continuity relations of the tangential component of the electric and magnetic fields lead to :

$$Z'_{j-1} = Z_j \quad (67)$$

and the homogeneity of the materials leads to :

$$z'_j = z_j. \quad (68)$$

From relation (63) it follows that :

$$\alpha_j = \alpha'_j \exp\left(\frac{2 \cdot i \cdot d_j \cdot k_{\perp j}}{\lambda}\right). \quad (69)$$

The set of relations (65) to (69) forms the recursive procedure.

The computational procedure starts at the bottom of the stack, by setting $\alpha_n = 0$ and works backward to the top of the pile to give finally α_1 and the reflectance $\mathcal{R} = \alpha_1 \cdot \alpha_1^*$.

4. Microscopic approach.

The approaches presented previously are completely equivalent, in the sense that they give the same numerical results, provided the calculations have been carried out with the same degree of approximation and precision. This situation is not surprising, since these methods have the same physical foundation (i.e., the dynamical theory in absorbing media) and the parameters have identical properties, in particular the materials are considered as continuous. If the materials are structured on an atomic scale, for instance if they are in a crystalline form or if the thicknesses of the layers are only of a few atomic radii, a microscopic approach may be relevant. So Litzmann *et al.* emphasize [29] that the T.E. reflectance calculated within the framework of a macroscopic model is for small angles of incidence less than the reflectance deduced from their microscopic approach taking into account the discrete nature of the dielectric materials. Their model of a dielectric slab assumes that the medium is a system of classical dipoles having no permanent dipole moment, fixed on the lattice points of a cubic lattice. This *a priori* microstructure appears questionable for the films obtained in practice in the composition of the X-UV multilayered mirrors, produced up to

now. The texture seems to be rather amorphous or polycrystalline. This model could be relevant for epitaxial 2D-superlattices. For ultrathin films, a microscopic theory has been recently published [30].

5. Imperfection effects.

The periodic bilayered mirrors manufactured in practice differ from the ideal structures studied in the previous sections on essentially three accounts :

- the thicknesses are different from the nominal values, that is from the values ideally required ;
- the interfaces are not perfectly flat and sharp, but more or less diffuse giving rise to the so-called interfacial roughness ;
- the layers are not homogeneous but can present local variations in composition, porosities, inclusions of elements foreign to the nominal composition.

The characteristics of the latter imperfections are essentially dependent on the method and the conditions of manufacture. Provided that the composition of the layers can be modeled by an index profile, the B.K.W method (see Sect. 1) can profitably be used. The thickness errors, if they are not systematic, can be treated by a statistical approach. Incidentally it is important to establish a distinction to set clearly the problem of the statistical treatment for the various imperfections relevant to random processes. A statistical problem needs a preliminary definition of the statistical universes involved. We can distinguish two distinct statistical universes :

i) the first universe is defined from the set of the N layers of a given mirror, provided the number N is sufficient. This notion is easy to understand in the case of periodic stacks but would need a more precise definition in the others cases. One can then define the statistical moments of first, second... orders of the different characteristic quantities q of layers ; for instance : thickness, refractive index, and even the quantities of statistical nature as the r.m.s. and the autocorrelation length of the interfacial roughness. We set :

$$\bar{q} = \frac{\sum_{i=1}^N q_i}{N} \quad (70a)$$

$$\bar{q}^2 = \frac{\sum_{i=1}^N q_i^2}{N} \quad (70b)$$

$$\bar{q}^\alpha = \frac{\sum_{i=1}^N q_i^\alpha}{N} \quad (70c)$$

where the index runs over the set of the N layers ;

ii) the second universe is defined from the set of the M samples admitted to have been manufactured

with identical conditions. One can define the statistical moments of the different characteristic quantities Q of the samples ; for instance the thickness of the i -th layer of the j -th sample. We define :

$$\langle Q_i \rangle = \frac{\sum_{j=1}^N Q_{i,j}}{M} \quad (71a)$$

$$\langle Q_i^2 \rangle = \frac{\sum_{j=1}^N Q_{i,j}^2}{M} \quad (71b)$$

$$\langle Q_i^\alpha \rangle = \frac{\sum_{j=1}^N Q_{i,j}^\alpha}{M} \quad (71c)$$

where the index j runs over the set of the M samples. The symbol $\langle \rangle$ stands for the ensemble average over the samples of a *given* production, while the symbol $\bar{}$ stands for the average over the layers of a given mirror.

Consequently the theorician has to deal with two different problems : either to determine the performances of a given sample when disposing of statistical data of the first universe either to compute the different statistical moments of quantities evaluating the performances of samples obtained from a given production, when disposing of statistical data of the second universe.

A global treatment of the thickness errors and the interfacial roughness may be better since their influences are not *a priori* uncorrelated. Nevertheless this is a task beyond the scope of this paper.

To account phenomenologically for the different imperfection effects, it has become usual to define an effective r.m.s. σ_e entering a Debye-Waller corrective factor S :

$$\mathcal{R}_E = S \cdot \mathcal{R}_I \quad (72)$$

where \mathcal{R}_I is the reflectance affected by the imperfections, \mathcal{R}_E is the ideal reflectance and

$$S = \exp(-4 \cdot k_\perp^2 \cdot \sigma_e^2) \quad (73)$$

However this manner of characterizing the sample quality can lead to inconsistencies since the value of σ_e seems to depend on the wavelength and the glancing angle. On the other hand, as mentioned by Spiller and Rosenbluth [19] the influences of the two imperfections are both lumped into σ_e and cannot be distinguished. In the following, we discuss separately the influence of thickness errors and interfacial roughness.

5.1 THICKNESS ERRORS. — When one considers the various methods of production, one is led to distinguish between the so-called cumulative errors and the compensated errors. Thus Spiller *et al.* [31],

Chauvineau *et al.* [32] monitor *in situ* the absolute positions of the interfaces by measuring the extrema of reflectance of the structure during the deposition. With this method, the absolute positions of the interfaces are by principle close to the nominal positions and the errors do not accumulate. Others methods control in fact the thicknesses of the layers, instead of the absolute positions which give rises to cumulative errors. In this case, the performance of the mirrors runs the risk of being considerably deteriorated by a large number of layers.

To illustrate the influence of these errors, we adopt a kinematic approach assuming that the transmitted wave is not very depleted. Moreover, we suppose that the Bragg law is fulfilled within the phase errors resulting from the uncertainty in the interface positions. The amplitude reflected by N bilayers is then given by :

$$\rho = r_{bi} \sum_{q=1}^N \exp(i \cdot \varphi_q) \quad (74)$$

where r_{bi} is the coefficient reflection of a bilayer and φ_q the phase delay coming from the q -th bilayer. For the sake of simplicity, we have not distinguished the two kinds of interface.

When the Bragg law is nearly satisfied :

$$\varphi_q = 2 \cdot p \cdot \pi + \delta \varphi_q \quad (75a)$$

and

$$\rho = r_{bi} \sum_{q=1}^N \exp(i \cdot \delta \varphi_q) \quad (75b)$$

Let us consider firstly the case of non-cumulative errors. Then relation (75b) can be considered as an arithmetic mean value :

$$\rho = r_{bi} \cdot N \frac{\sum_{q=1}^N \exp(i \cdot \varphi_q)}{N} \quad (76)$$

Provided that N is very large and $\delta \varphi_q$ sufficiently small, the arithmetic mean can be assimilated to the expectation value calculated in the statistical universe of the layers :

$$\rho \simeq r_{bi} \cdot N \overline{\exp(i \cdot \delta \varphi_q)} \quad (77)$$

Assuming that the distribution of $\delta \varphi_q$ is Gaussian, then :

$$\overline{\exp(i \cdot \delta \varphi_q)} = \exp\left(-\frac{1}{2} \delta \varphi^2\right) \quad (78)$$

that means that the coefficient ρ in presence of compensated errors is merely the ideal coefficient affected by an amplitude Debye-Waller factor :

$$\rho = r_{bi} \cdot N \exp\left(-\frac{1}{2} \delta \varphi^2\right) \quad (79a)$$

The reflectance $\mathcal{R} = \rho \cdot \rho^*$ is then :

$$\mathcal{R} = r_{\text{bi}}^2 \cdot N^2 \cdot \exp(-\overline{\delta\varphi^2}). \quad (79b)$$

Let us consider the ensemble average of the coefficient ρ in the sample statistical universe :

$$\langle \rho \rangle = r_{\text{bi}} \sum_{q=1}^M \langle \exp(i \cdot \delta\varphi_q) \rangle. \quad (80)$$

For a Gaussian distribution :

$$\langle \rho \rangle = r_{\text{bi}} \sum_{q=1}^M \exp\left(-\frac{1}{2} \langle \delta\varphi_q^2 \rangle\right). \quad (81)$$

Since the errors are non-cumulative, it is reasonable to consider that :

$$\langle \delta\varphi_q^2 \rangle = \langle \delta\varphi^2 \rangle \quad (82)$$

and consequently :

$$\rho \approx \langle \rho \rangle. \quad (83)$$

The ensemble average $\langle \mathcal{R} \rangle$ of the reflectance is :

$$\langle \rho\rho^* \rangle = |r_{\text{bi}}|^2 \left\langle \sum_{j=1}^N \sum_{k=1}^N \exp[i \cdot (\delta\varphi_j - \delta\varphi_k)] \right\rangle \quad (84)$$

that is, with the same assumptions :

$$\langle \mathcal{R} \rangle = |r_{\text{bi}}|^2 [N^2 \cdot \exp(-\langle \delta\varphi^2 \rangle) - N \cdot (1 - \exp(-\langle \delta\varphi^2 \rangle))] \quad (85)$$

It should be emphasize that $\langle \mathcal{R} \rangle$ is the expectation value in the sample statistical universe. This quantity enables us to predict the reflectance of a given mirror if the normalized variance $\text{var}(\rho)/\langle \rho \cdot \rho^* \rangle$ is small enough.

Indeed we know according to equation (82) that if \mathcal{R} is significant, then :

$$\frac{\text{var}(\rho)}{\langle \rho\rho^* \rangle} = 1 - \frac{\rho\rho^*}{\langle \rho\rho^* \rangle}. \quad (86)$$

Since

$$\frac{\text{var}(\rho)}{\langle \rho\rho^* \rangle} = \frac{1 - \exp(-\langle \delta\varphi^2 \rangle)}{N \cdot \exp(-\langle \delta\varphi^2 \rangle)} \quad (87)$$

it results that :

$$\langle \mathcal{R} \rangle = \rho\rho^* \quad (88)$$

provided that N is sufficiently large even if $\langle \delta\varphi^2 \rangle$ is not very small. If the term $N(1 - \exp(-\langle \delta\varphi^2 \rangle))$ is required to obtain a correct estimation of the ensemble average $\langle \mathcal{R} \rangle$ from relation (85), then this average is inadequate to predict the reflectance of a given mirror. It can be only used to estimate the expected value of the reflectance for a given pro-

duction with a degree of confidence determined by the magnitude of $\langle \delta\varphi^2 \rangle$.

The case of the cumulative errors is more problematic in the sense that the estimation of the reflectance in the layer statistical universe is not straightforward. Nevertheless it is natural to extend to the present case the validity of the result found for the latter case ; if \mathcal{R} is still significant in presence of thickness errors, it can be obtained from the ensemble average $\langle \mathcal{R} \rangle$.

A somewhat tedious calculation yields :

$$\langle \mathcal{R} \rangle = |r_{\text{bi}}|^2 \times \left[N + \sum_{k=1}^N 2 \cdot (N - k) \cdot \exp(-\langle \delta\varphi^2 \rangle) \right] \quad (89)$$

while

$$\langle \rho \rangle = r_{\text{bi}} \frac{1 - \exp(-N \langle \delta\varphi^2 \rangle)}{1 - \exp(-\langle \delta\varphi^2 \rangle)}. \quad (90)$$

When the number of bilayers N is large but $\langle \delta\varphi^2 \rangle$ is sufficiently small so that relations (89), (90) can be expanded to the second order with respect to $\langle \delta\varphi^2 \rangle$, the ensemble averages $\langle \rho \rangle$ and $\langle \mathcal{R} \rangle$ are given by :

$$\langle \rho \rangle = N \cdot r_{\text{bi}} \left(1 - \frac{N}{2} \langle \delta\varphi^2 \rangle \right) \quad (91)$$

and

$$\langle \mathcal{R} \rangle = N^2 \cdot |r_{\text{bi}}|^2 \left(1 - \frac{1}{3} \langle \delta\varphi^2 \rangle \right). \quad (92)$$

In these conditions, the normalized variance is :

$$\frac{\text{var}(\rho)}{\langle \rho\rho^* \rangle} = \frac{2}{3} N \cdot \langle \delta\varphi^2 \rangle. \quad (93)$$

Accordingly, a correct evaluation of the reflectance in presence of cumulative errors by the means of $\langle \mathcal{R} \rangle$ would need a negligible corrective term $N \cdot \langle \delta\varphi^2 \rangle$ in relations (91), (92).

Finally let us consider, the two limiting cases

i) $\langle \delta\varphi^2 \rangle \rightarrow 0$ and ii) $\langle \delta\varphi^2 \rangle \rightarrow \infty$.

i) In the first case, and for the two kinds of errors

$$\langle \rho \rangle = N \cdot r_{\text{bi}}, \quad (94a)$$

$$\langle \mathcal{R} \rangle = N^2 |r_{\text{bi}}|^2. \quad (94b)$$

This result is expected, since the reflection from each bilayer is correlated and the amplitudes are additive.

ii) In the second case, and for the two kinds of errors :

$$\langle \rho \rangle = 0, \quad (95a)$$

$$\langle \mathcal{R} \rangle = N |r_{\text{bi}}|^2. \quad (95b)$$

The reflections are not correlated, and the intensities only are additive.

5.2 INTERFACIAL ROUGHNESS EFFECTS. — When an interface is rough, scattered radiation in the whole space may be induced. Nevertheless in the X-UV region, the total integrated scattered radiation remains generally localized in the vicinity of the specular direction, or is negligible. Thus one expects that the main consequence of the interfacial roughness is to reduce the Bragg reflectance and to increase the transmission, the broadening of the Bragg peaks being relatively limited. The rough interface can be in first approximation considered as a stratified transition layer. The z -dependence of the refractive index within the layer is schematically given in figure 6 ; the index presents a continuous and gradual variation from the nominal value in the 2 medium to the corresponding value in the 1 medium. The thickness of the transition layer can be used to characterize the roughness magnitude or alternatively can be related to the r.m.s. σ of the roughness heights within a statistical approach of the roughness.

A hyperbolic tangential function or the error function erf [33] can be used in practice. The erf is interesting because of its behavior with regard to the Fourier transform. The problem is then reduced to the determination of the wave propagation in a stratified medium with a given index profile and can be in practice treated by the W-K-B method (see sect. 1.2). To avoid this somewhat cumbersome approach, we account for the roughness by a homogeneous film with an index averaged between the

two extreme materials, and a thickness close to the r.m.s. This approach can seem to be oversimplified ; nevertheless it is instructive to treat the problem of a stratified transition layer. To solve the problem of the homogeneous transition layer, we adopt the matricial formalism with initially the U, V representation since, as shown before, the passage matrix for an ideal interface is the identity. To realize the perturbative transition layer, we withdraw a thickness d from each material (2 and 1), then we insert between the two media a film of thickness $2d$. The passage matrix is then given by the matricial product.

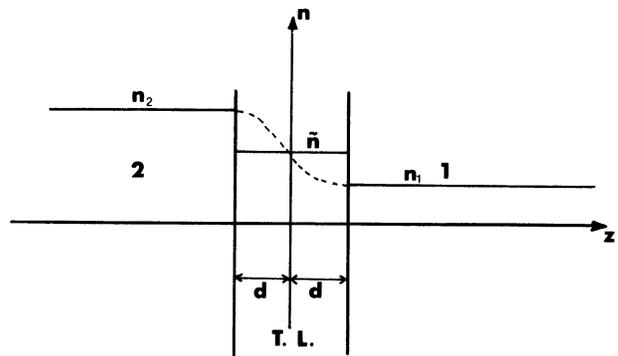


Fig. 7. — Model of the interfacial roughness ; a homogeneous transition layer (T. L.) with the averaged refractive in index $n = \bar{n} (n_1, n_2)$ and the thickness $2d$ is used to describe the roughness.

$$\begin{pmatrix} \cos(k_{\perp 2} d) & -\frac{ik_0}{k_{\perp 2}} \sin(k_{\perp 2} d) \\ -\frac{ik_{\perp 2}}{k_0} \sin(k_{\perp 2} d) & \cos(k_{\perp 2} d) \end{pmatrix} \begin{pmatrix} \cos(k_{\perp 1} d) & \frac{ik_0}{k_{\perp 1}} \sin(k_{\perp 1} d) \\ -\frac{ik_{\perp 1}}{k_0} \sin(k_{\perp 1} d) & \cos(k_{\perp 1} d) \end{pmatrix} \times \begin{pmatrix} \cos(k_{\perp} 2d) & \frac{ik_0}{k_{\perp}} \sin(k_{\perp} 2d) \\ \frac{ik_{\perp}}{k_0} \sin(k_{\perp} 2d) & \cos(k_{\perp} 2d) \end{pmatrix} \times \begin{pmatrix} \cos(k_{\perp 2} d) & -\frac{ik_0}{k_{\perp 2}} \sin(k_{\perp 2} d) \\ -\frac{ik_{\perp 2}}{k_0} \sin(k_{\perp 2} d) & \cos(k_{\perp 2} d) \end{pmatrix} \quad (96)$$

To carry out the calculations, we expand the cosinus and sinus functions to the third order with respect to d ; it follows that :

$$\begin{pmatrix} 1 - \frac{k_{\perp 2}^2 d^2}{2} & -i \cdot k_0 d \\ -i \frac{k_{\perp 2}^2 d}{k_0} & 1 - \frac{k_{\perp 2}^2 d^2}{2} \end{pmatrix} \times \begin{pmatrix} 1 - \frac{k_{\perp 1}^2 d^2}{2} & i \cdot k_0 d \\ i \frac{k_{\perp 1}^2 d}{k_0} & 1 - \frac{k_{\perp 1}^2 d^2}{2} \end{pmatrix} \times \begin{pmatrix} 1 - \frac{k_{\perp}^2 d^2}{2} & -i \cdot k_0 d \\ -i \frac{k_{\perp}^2 d}{k_0} & 1 - \frac{k_{\perp}^2 d^2}{2} \end{pmatrix} \quad (97)$$

then after a tedious matrix multiplication

$$\begin{pmatrix} 1 - \frac{d^2}{2} (k_{\perp 2}^2 - k_{\perp 1}^2) & 0 \\ i \frac{d}{k_0} (2 \cdot k_{\perp}^2 - k_{\perp 1}^2 - k_{\perp 2}^2) & 1 + \frac{d^2}{2} (k_{\perp 2}^2 - k_{\perp 1}^2) \end{pmatrix} \quad (98)$$

If the averaged index n is judiciously chosen : $n = \bar{n} = \sqrt{\frac{n_1^2 + n_2^2}{2}}$ the latter matrix takes the simple diagonal form :

$$\begin{pmatrix} 1 - \frac{d^2}{2} (k_{\perp 2}^2 - k_{\perp 1}^2) & 0 \\ 0 & 1 + \frac{d^2}{2} (k_{\perp 2}^2 - k_{\perp 1}^2) \end{pmatrix}. \quad (99)$$

It appears that the two extreme media contribute through the normal components of the wavevectors to the transition matrix. To return to the (T, R) representation we use the pseudo-similarity transformation (see sect. 2) :

$$\frac{1}{2} \begin{pmatrix} 1 & \frac{k_0}{k_{\perp 2}} \\ 1 & -\frac{k_0}{k_{\perp 2}} \end{pmatrix} \times \begin{pmatrix} 1 - \frac{d^2}{2} (k_{\perp 2}^2 - k_{\perp 1}^2) & 0 \\ 0 & 1 + \frac{d^2}{2} (k_{\perp 2}^2 - k_{\perp 1}^2) \end{pmatrix} \times \begin{pmatrix} 1 & \frac{1}{k_0} \\ \frac{k_{\perp 1}}{k_0} & -\frac{k_{\perp 1}}{k_0} \end{pmatrix}. \quad (100)$$

that is,

$$\frac{1}{2} \begin{pmatrix} \frac{k_{\perp 2} + k_{\perp 1}}{k_{\perp 2}} \left[1 - \frac{d^2}{2} (k_{\perp 2} - k_{\perp 1})^2 \right] \frac{k_{\perp 2} - k_{\perp 1}}{k_{\perp 2}} \left[1 - \frac{d^2}{2} (k_{\perp 2} + k_{\perp 1})^2 \right] \\ \frac{k_{\perp 2} - k_{\perp 1}}{k_{\perp 2}} \left[1 - \frac{d^2}{2} (k_{\perp 2} + k_{\perp 1})^2 \right] \frac{k_{\perp 2} + k_{\perp 1}}{k_{\perp 2}} \left[1 - \frac{d^2}{2} (k_{\perp 2} - k_{\perp 1})^2 \right] \end{pmatrix}. \quad (101)$$

If we divide the coefficients of the matrix by

$$\frac{k_{\perp 2} + k_{\perp 1}}{k_{\perp 2}} \left[1 - \frac{d^2}{2} (k_{\perp 2} - k_{\perp 1})^2 \right]$$

and we introduce the Fresnel coefficients $r_{2,1}$ and $t_{2,1}$, it yields :

$$\frac{1 - \frac{d^2}{2} (k_{\perp 2} - k_{\perp 1})^2}{t_{2,1}} \begin{bmatrix} 1 & r_{2,1}(1 - 2 \cdot d^2 k_{\perp 1} k_{\perp 2}) \\ r_{2,1}(1 - 2 \cdot d^2 k_{\perp 1} k_{\perp 2}) & 1 \end{bmatrix}. \quad (102)$$

The expressions $1 - 2 \cdot d^2 k_{\perp 1} k_{\perp 2}$ and $1 - \frac{d^2}{2} (k_{\perp 2} - k_{\perp 1})^2$ can be respectively considered as the first terms of the expansions of $\exp[-2 \cdot d^2 k_{\perp 1} k_{\perp 2}]$ and $\exp\left[-\frac{d^2}{2} (k_{\perp 2} - k_{\perp 1})^2\right]$ so that the transition matrix can be rewritten :

$$M_t = \frac{1}{t_{2,1} \exp\left[+\frac{d^2}{2} (k_{\perp 2} - k_{\perp 1})^2\right]} \times \begin{bmatrix} 1 & r_{2,1} \exp[-2 \cdot d^2 k_{\perp 1} k_{\perp 2}] \\ r_{2,1} \exp[-2 \cdot d^2 k_{\perp 1} k_{\perp 2}] & 1 \end{bmatrix}. \quad (103)$$

This matrix takes the place of the Fresnel matrix given by relation (36), in the case of a rough boundary. It shows that the reflection coefficient is decreased by a Debye-Waller type factor where the usual square of the wavenumber is replaced by the product $k_{1\perp} \cdot k_{2\perp}$, while the transmission coefficient is increased by the factor :

$$\exp\left[+\frac{d^2}{2} (k_{\perp 2} - k_{\perp 1})^2\right].$$

This formalism can be profitably used to analyse the

roughness of each interface from X-ray grazing incidence reflectivity measurements [34].

Conclusion and perspective.

Within the macroscopic framework of electromagnetism in continuous media, the propagation of a wave in a stratified structure can be treated either from a linear differential equation of the second order whose solution is a wave function, or from a system of two linear differential equations of the first

order, whose solution is a propagator represented by a 2×2 matrix.

Fundamentally the two approaches are equivalent. Nevertheless for the case of periodic structures as the interference mirrors, the study of the second order equation is fruitful under the assumption of an infinite structure. Indeed it is then possible to introduce the Hill determinant leading to an elegant formulation for the wave propagation and giving easily a generalization of the Bragg conditions. This approach is conceptually attractive, though for the absorbing media as in the X-UV spectrum the introduction of complex refractive index is tricky.

Our review is non exhaustive ; for instance the powerful Green methods appropriate to describe the microscopic processes, which have been used by Croce [34] are not presented since it would need

mathematical developments beyond the scope of the paper.

On the other hand, we have implicitly assumed that the radiation is generated outside the multilayered structure. The general approach given in section 1 makes it possible to expect attractive phenomena when the radiation is generated inside the structure. Indeed a radiation of wavelength λ stimulated within an appropriate material of a bilayered structure will undergo resonant oscillations provided the period d of the structure is tuned to the wavelength λ according to the Bragg law. It results the opportunity to obtain a X-UV amplifying multilayered medium offering an alternative to the usual Fabry-Perot resonator. The pumping procedure in this distributed X-UV laser could be achieved by an external incoherent source.

Appendice A.

The dispersion relation

$$\sin^2 \left(\frac{K \cdot d}{2} \right) = \frac{1}{1-r^2} \sin^2 \left(k_0 J^+ \frac{d}{2} \right) - \frac{r^2}{1-r^2} \sin^2 \left(k_0 J^- \frac{d}{2} \right) \quad (\text{A.1})$$

with

$$J^+ = \frac{n_1 \cdot d_1 \cdot \sin(\theta_1) + n_2 \cdot d_2 \cdot \sin(\theta_2)}{d} \quad J^- = \frac{n_1 \cdot d_1 \cdot \sin(\theta_1) - n_2 \cdot d_2 \cdot \sin(\theta_2)}{d}$$

gives, when the Bragg condition (18) is satisfied :

$$\sin^2 \left(k_0 J^+ \frac{d}{2} \right) = r^2 \sin^2 \left(k_0 J^- \frac{d}{2} \right) \quad \text{if} \quad K \cdot d = 2 \cdot l \cdot \pi \quad (\text{A.2})$$

and

$$\sin^2 \left(k_0 J^+ \frac{d}{2} \right) = 1 - r^2 \cos^2 \left(k_0 J^- \frac{d}{2} \right) \quad \text{if} \quad K \cdot d = (2 \cdot l + 1) \cdot \pi \quad (\text{A.3})$$

l being a positive integer.

Since in X-UV region the refractive index is close to unity, then $J^+ = \sin(\theta)$. Therefore the upper and lower limits k_0^+ and k_0^- of the Bragg gaps are approximately given by :

$$k_0^\pm = \frac{1}{J^+ d} \left(p \cdot \pi \pm 2 \cdot \sin^{-1} \left(r \cdot \sin \left(\frac{J^-}{J^+} p \frac{\pi}{2} \right) \right) \right) \quad \text{if} \quad p = 2 \cdot l \quad (\text{A.4})$$

and

$$k_0^\pm = \frac{1}{J^+ d} \left(p \cdot \pi \pm 2 \cdot \sin^{-1} \left(r \cdot \sin \left(\frac{J^-}{J^+} p \frac{\pi}{2} \right) \right) \right) \quad \text{if} \quad p = 2 \cdot l + 1. \quad (\text{A.5})$$

Since in X-UV region the coefficient r is very small (typically 10^{-6}) only the first system in the expansion of \sin^{-1} is required to give the gapwidth.

$$\Delta k_0 = \frac{4}{d \cdot \sin(\theta)} \left| r \cdot \sin \left(\frac{J^-}{J^+} p \frac{\pi}{2} \right) \right| \quad \text{if} \quad p = 2 \cdot l \quad (\text{A.6})$$

$$\Delta k_0 = \frac{4}{d \cdot \sin(\theta)} \left| r \cdot \cos \left(\frac{J^-}{J^+} p \frac{\pi}{2} \right) \right| \quad \text{if} \quad p = 2 \cdot l + 1. \quad (\text{A.7})$$

Noting that $\frac{J^-}{J^+} \simeq 2 \cdot \gamma - 1$, by trigonometry we obtain :

$$\Delta k_0 = \frac{4}{d \cdot \sin(\theta)} |r \cdot \sin(p \cdot \gamma \cdot \pi)|. \quad (\text{A.8})$$

Appendix B.

EIGENELEMENTS OF THE BILAYER MATRIX M_{bi} AND CHEBYCHEV IDENTITY. — The bilayer matrix M_{bi} is written in the general form :

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}. \tag{B.1}$$

Let us denote by S its trace

$$S = C_{11} + C_{22} \tag{B.2}$$

M_{bi} is unitary, i.e.,

$$\det (M_{bi}) = 1. \tag{B.3}$$

The eigenvalues P_+ , P_- of M_{bi} are the roots of the characteristic equation :

$$P^2 - P \cdot S + 1 = 0 \tag{B.4}$$

that is,
$$P_{\pm} = \frac{S \pm \sqrt{S^2 - 4}}{2}. \tag{B.5}$$

Obviously
$$P_+ + P_- = S \tag{B.6}$$

$$P_+ \cdot P_- = 1. \tag{B.7}$$

The normalized eigenvectors Z_+ , Z_- belonging respectively to P_+ , P_- are given by :

$$Z_+ = \begin{pmatrix} V_+ \\ W_+ \end{pmatrix}, \tag{B.8a}$$

$$Z_- = \begin{pmatrix} V_- \\ W_- \end{pmatrix} \tag{B.8b}$$

where

$$V_{\pm} = \frac{C_{12}}{\sqrt{C_{12} + (P^{\pm} - C_{11})^2}}, \tag{B.9a}$$

$$W_{\pm} = \frac{P^{\pm} - C_{11}}{\sqrt{C_{11} + (P^{\pm} - C_{11})^2}}. \tag{B.9b}$$

We define the Fresnel eigencoefficients of reflection ρ_+ and ρ_- by :

$$\rho_{\pm} = \frac{W_{\pm}}{V_{\pm}}. \tag{B.10}$$

it follows that :

$$\rho_{\pm} = \frac{P_{\pm} - C_{11}}{C_{12}}. \tag{B.11}$$

These coefficients are the roots of the trinomial equation

$$\rho^2 - \tilde{S} \cdot \rho + \tilde{P} = 0 \tag{B.12}$$

with
$$\tilde{S} = \frac{C_{22} - C_{11}}{C_{12}} \tag{B.13}$$

and
$$\tilde{P} = -\frac{C_{21}}{C_{12}}. \tag{B.14}$$

By expliciting C_{ij} , one obtains :

$$\tilde{S} = \exp(i \cdot \varphi_2) \frac{\sin(\Phi)}{r \cdot \sin(\varphi_1)} \tag{B.15}$$

$$\tilde{P} = \exp(2 \cdot i \cdot \varphi_2). \tag{B.16}$$

Consequently

$$\rho_{\pm} = \exp(i \cdot \Phi_2) [\mathcal{A} \pm \sqrt{\mathcal{A}^2 - 1}] \tag{B.17}$$

with
$$\mathcal{A} = \frac{\sin(\Phi)}{2 \cdot r \cdot \sin(\varphi_1)}. \tag{B.18}$$

Chebyshev identity. — The matrix M_{bi} is related to the diagonal matrix D_{bi} by the similarity relation

$$M_{bi} = S^{-1} \times D_{bi} \times S \tag{B.19}$$

with
$$D_{bi} = \begin{bmatrix} P_+ & 0 \\ 0 & P_- \end{bmatrix} \tag{B.20}$$

S is constructed from the elements of the eigenvectors Z_+ , Z_-

$$S = \frac{1}{\sqrt{V_+ \cdot W_- - V_- \cdot W_+}} \begin{pmatrix} W_- & -V_- \\ -W_+ & V_+ \end{pmatrix} \tag{B.21}$$

and

$$S^{-1} = \frac{1}{\sqrt{V_+ \cdot W_- - V_- \cdot W_+}} \begin{pmatrix} V_+ & V_- \\ W_+ & W_- \end{pmatrix}. \tag{B.22a}$$

To obtain the N -th power of M_{bi} , it is convenient to use the relation :

$$(M_{bi})^N = (S^{-1} D_{bi} S)^N = S^{-1} D_{bi}^N S. \tag{B.22b}$$

If one notes that $P_{\pm} = \exp(\pm iK \cdot d)$ and one explicites S and S^{-1} , the matricial product gives :

$$(M_{bi})^N = \begin{pmatrix} C_{11} U_{N-1}(K \cdot d) - U_{N-2}(K \cdot d) & C_{12} U_{N-1}(K \cdot d) \\ C_{21} U_{N-1}(K \cdot d) & C_{22} U_{N-1}(K \cdot d) - U_{N-2}(K \cdot d) \end{pmatrix} \tag{B.23}$$

with

$$U_N(x) = \frac{\sin[(N+1) \cdot x]}{\sin(x)}. \tag{B.24}$$

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