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Coherent and Incoherent Reflection and Transmission of Multilayer Structures

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Abstract. The complex-amplitude reflection and transmission coefficients r and t of a pile of films are represented as a product of matrices. The matrices describe the transformation of two plane waves travelling in opposite directions between the films, and their development within the films.
If one of the films is significantly thicker than the other layers (e.g., several films on a substrate), the calculated reflectance $R=rr^*$ and transmittance $T\sim tt^*$ show narrow Fabry-Perot oscillations which, in a lot of cases, are not observed in the experiment. Since the matrix method is equivalent to the representation of the amplitudes r and t as a coherent superposition of multiple reflected waves within the thick slab, we are able to suppress, in the calculation, the interference within this thick film by adding the absolute squares of the partial waves corresponding to an incoherent treatment. This procedure is shorter and more simple than averaging over an appropriate interval of frequency or thickness, which, in most cases, leads to the same results.

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A method often chosen to determine the optical constants of solid-state materials is the measurement of the intensity of light reflected and transmitted by certain samples [1].
To obtain a transmitted signal in spectral regions where high absorption occurs, sufficiently thin samples have to be prepared. Often, this is only possible as a film on a supporting substrate. In other cases, it is necessary to take into account a transition layer between substrate and film and/or an oxide cover on the surface of the film. Also, films can cover both surfaces of a substrate, e.g. thermally oxidized silicon wafers. Thus we have to analyse a system of several layers. As examples see [2].
In Sect. 1 we present a method to calculate the complex-amplitude reflection and transmission coefficients r and t for a pile of L parallel faced layers. If one layer of the pile is more than several wavelengths thick and sufficiently transparent, narrow Fabry-Perot oscillations may occur in the reflectance $R=rr^*$ and in the transmittance $T\sim tt^*$. These oscillations are usually not resolved in the measurements. This indicates that the assumptions for the model calculation, such as plane and parallel surfaces and the monochromatic light source, are not realistic.
In Sect. 2.1 we present a procedure which is able to turn off the interference within a thick layer; this concept is based on the idea of coherent and incoherent multiple reflections.
The extension of the procedure to an arbitrary number of thick films will be given in Sect. 2.2. Finally, this "concept of multiple reflection" is compared with the "method of averaging".

1. Transfer Matrix of a System of Parallel Faced Layers

A plane electromagnetic wave

$$\mathbf{E}_i(\mathbf{r},t)=\mathbf{E}_i\exp[\mathrm{i}(\mathbf{k}_i\cdot\mathbf{r}-\omega t)]$$

is incident on a pile of L parallel faced layers (Fig. 1). Let the optical properties of each layer be isotropic and

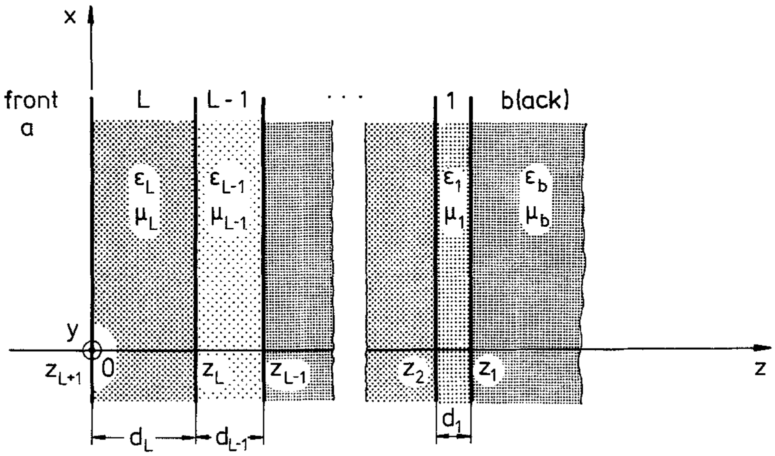

Fig. 1. The pile of layers and the co-ordinates used throughout the text

homogeneous and be described by a dielectric function $\varepsilon(\omega)$ and a magnetic permeability $\mu(\omega)$. Then a reflected wave $\mathbf{E}_r(\mathbf{r}, t)$ and a transmitted wave $\mathbf{E}_t(\mathbf{r}, t)$ exist.

We consider the case of s-polarization (TE wave), i.e., the electric field $\mathbf{E} = (0, E, 0)$ is parallel to the interfaces, also for oblique incidence. If the light is p-polarized (TM wave) we consider the field $\mathbf{H} = (0, H, 0)$ which is now parallel to the interfaces; the corresponding modifications in the formulae are given in the appendix.

We describe the electric field in any layer as a superposition of two plane waves. E.g., for layer l (α: angle of incidence)

$$\begin{aligned} E_l(x,z,t) &= [E_l^{(+)}(z) + E_l^{(-)}(z)] \\ &\quad \cdot \exp\left[\mathrm{i}\left(\frac{\omega}{c} x \sin\alpha - \omega t\right)\right] \\ &= \left[E_l^{(+)} \exp\left(\mathrm{i}\frac{\omega}{c}\tilde{N}_l z\right)\right. \\ &\quad \left. + E_l^{(-)} \exp\left(-\mathrm{i}\frac{\omega}{c}\tilde{N}_l z\right)\right] \\ &\quad \cdot \exp\left[\mathrm{i}\left(\frac{\omega}{c} x \sin\alpha - \omega t\right)\right]. \end{aligned} \tag{1}$$

The generalized complex index of refraction

$$\tilde{N} = N + \mathrm{i}K = \sqrt{\varepsilon\mu - \sin^2\alpha} \tag{2}$$

reduces to the complex index of refraction for normal incidence.

To calculate the reflection and transmission we apply a matrix method [3] which consists of successive application of two transfer operations (Fig. 2):

(a) The transformation of the fields $E^{(+)}$ and $E^{(-)}$ across the interface between two layers, and

(b) the transformation through the layer, from right to left

$$\begin{aligned} \begin{Bmatrix} E_l^{(+)} \\ E_l^{(-)} \end{Bmatrix}_{z_{l+1}} &= \begin{Bmatrix} \phi_l^{-1} & 0 \\ 0 & \phi_l \end{Bmatrix} \\ &\quad \cdot \begin{Bmatrix} 1/\tau_{l,l-1} & \varrho_{l,l-1}/\tau_{l,l-1} \\ \varrho_{l,l-1}/\tau_{l,l-1} & 1/\tau_{l,l-1} \end{Bmatrix} \cdot \begin{Bmatrix} E_{l-1}^{(+)} \\ E_{l-1}^{(-)} \end{Bmatrix}_{z_l}, \end{aligned} \tag{3}$$

where

$$\phi_l = \exp\left(\mathrm{i}\frac{\omega}{c}\tilde{N}_l d_l\right) \equiv \exp\left(\mathrm{i}\frac{\omega}{c}N_l d_l - \frac{\omega}{c}K_l d_l\right), \tag{4}$$

where d_l is the thickness of layer l; and ϱ and τ are Fresnel's complex-amplitude reflection and transmission coefficients

$$\begin{aligned} \varrho_{l,l-1} &= \frac{\tilde{N}_l/\mu_l - \tilde{N}_{l-1}/\mu_{l-1}}{\tilde{N}_l/\mu_l + \tilde{N}_{l-1}/\mu_{l-1}}, \\ \tau_{l,l-1} &= \frac{2\tilde{N}_l/\mu_l}{\tilde{N}_l/\mu_l + \tilde{N}_{l-1}/\mu_{l-1}}. \end{aligned} \tag{5}$$

The product $\mathbf{T}$ of L matrices of type (3) (followed by the transformation through the surface of the pile at $z_{L+1} = 0$) yields the complete transfer of the fields from medium b to medium a, which is assumed to be vacuum throughout our paper,

$$\begin{Bmatrix} E_i \\ E_r \end{Bmatrix}_{z = z_{L+1} = 0} = \begin{Bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{Bmatrix} \cdot \begin{Bmatrix} E_t \\ 0 \end{Bmatrix}_{z = z_1}. \tag{6}$$

With the definition of the reflection and transmission coefficients

$$r_{ab} \stackrel{\text{def}}{=} \frac{E_r(z=0)}{E_i(z=0)}, \qquad t_{ab} \stackrel{\text{def}}{=} \frac{E_t(z=z_1)}{E_i(z=0)} \tag{7}$$

we rewrite (6) as

$$\begin{Bmatrix} 1 \\ r_{ab} \end{Bmatrix} = \begin{Bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{Bmatrix} \cdot \begin{Bmatrix} t_{ab} \\ 0 \end{Bmatrix} \tag{8}$$

and obtain

$$r_{ab} = T_{21}/T_{11}, \qquad t_{ab} = 1/T_{11}. \tag{9}$$

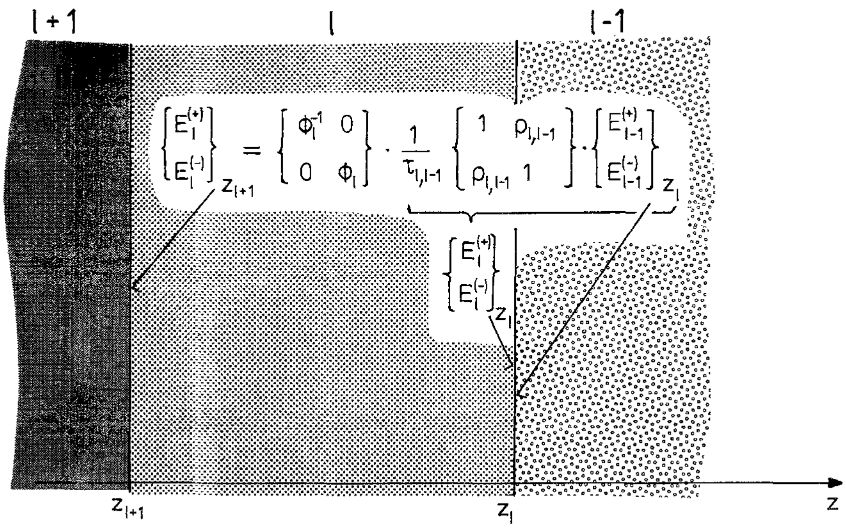

Fig. 2. The transformation of the waves $(E^{(+)}, E^{(-)})$ across the interface between layer $l-1$ and l and through the inside of layer l

The significance of the remaining matrix elements, T_{12} and T_{22}, appears if we consider the case where light is incident from the back b and emerges at the front a,

$$\begin{Bmatrix} 0 \\ t_{ba} \end{Bmatrix} = \begin{Bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{Bmatrix} \cdot \begin{Bmatrix} r_{ba} \\ 1 \end{Bmatrix}, \tag{10}$$

$$r_{ba} = -T_{12}/T_{11}, \qquad t_{ba} = (T_{11}T_{22} - T_{12}T_{21})/T_{11}.^{1} \tag{11}$$

Now the fields at the two boundaries of a pile can be connected by the reflection and transmission coefficients of that pile as follows

$$\begin{Bmatrix} E_i^{(+)} \\ E_i^{(-)} \end{Bmatrix} = \begin{Bmatrix} 1/t_{ij} & -r_{ji}/t_{ij} \\ r_{ij}/t_{ij} & (t_{ij}t_{ji} - r_{ij}r_{ji})/t_{ij} \end{Bmatrix} \cdot \begin{Bmatrix} E_j^{(+)} \\ E_j^{(-)} \end{Bmatrix}. \tag{12}$$

This representation will become essential in the next section.

2. Coherent Films and Incoherent Substrates

2.1. Substrate Between Two Piles of Films

Let us now consider the situation where one member of the pile of films, called substrate, needs a special treatment. We have in mind that the substrate destroys coherence between the neighbouring films to its right and left, but as long as we talk about complex amplitudes complete coherence is maintained [up to formula (15)].

We apply the formalism of the preceding section to the system medium a/pile 1/substrate/pile 2/medium b and obtain

$$\begin{Bmatrix} 1 \\ r_{ab} \end{Bmatrix} = \frac{1}{t_{as}} \begin{Bmatrix} 1 & -r_{sa} \\ r_{as} & t_{as}t_{sa} - r_{as}r_{sa} \end{Bmatrix} \cdot \frac{1}{\phi_s} \begin{Bmatrix} 1 & 0 \\ 0 & \phi_s^2 \end{Bmatrix} \cdot \frac{1}{t_{sb}} \begin{Bmatrix} 1 & -r_{bs} \\ r_{sb} & t_{sb}t_{bs} - r_{sb}r_{bs} \end{Bmatrix} \cdot \begin{Bmatrix} t_{ab} \\ 0 \end{Bmatrix}. \tag{13}$$

Evaluating the product of the three matrices, we can represent the transfer matrix $\mathbf{T}$ as

$$\mathbf{T} = \frac{1}{t_{ab}} \begin{Bmatrix} 1 & -r_{ba} \\ r_{ab} & t_{ab}t_{ba} - r_{ab}r_{ba} \end{Bmatrix} = \frac{1 - r_{sa}r_{sb}\phi_s^2}{t_{as}\phi_s t_{sb}} \cdot \begin{Bmatrix} 1 & -\left[r_{bs} + \dfrac{t_{bs}t_{sb}\phi_{sa}\phi_s^2}{1 - r_{sa}r_{sb}\phi_s^2} \right] \\ r_{as} + \dfrac{t_{as}t_{sa}r_{sb}\phi_s^2}{1 - \phi_{sa}\phi_{sb}\phi_2^2} & T_{22} \end{Bmatrix} \tag{14}$$

with

$$T_{22} = \frac{-r_{as}r_{bs} + (t_{as}t_{sa} - r_{as}r_{sa})\phi_s^2(t_{sb}t_{bs} - r_{sb}r_{bs})}{1 - r_{sa}r_{sb}\phi_s^2}.$$

Here, the transmission and reflection coefficients from front to back read

$$t_{ab} = \frac{t_{as}\phi_s t_{sb}}{1 - r_{sa}r_{sb}\phi_s^2}, \qquad r_{ab} = r_{as} + \frac{t_{as}t_{sa}r_{sb}\phi_s^2}{1 - r_{sa}r_{sb}\phi_s^2}. \tag{15}$$

They can be interpreted as the geometrical series of the field amplitudes of the partial waves reflected inside the substrate. This is well known in the case of a single film.

Up to now, we have merely rewritten the transfer matrix but we have given it a new interpretation. The advantage of this representation of multiple reflections is the fact that we can easily turn off coherence between

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[1] If back and front are built up by the same material then the determinant of the transfer matrix is unity, $\det(\mathbf{T}) = T_{11}T_{22} - T_{12}T_{21} = 1$, and $t_{ab} = t_{ba}$

the single-reflected amplitudes taking the absolute values of the complex coefficients t, r, and ϕ.
Thus we get for the reflectance and transmittance of this system with an incoherent substrate

$$R_{\mathrm{incoh}} = |r_{as}|^2 + \frac{|t_{as}t_{sa}r_{sb}|^2 \exp\left(-4\frac{\omega}{c}K_s d_s\right)}{1-|r_{sa}r_{sb}|^2 \exp\left(-4\frac{\omega}{c}K_s d_s\right)}, \tag{16}$$

$$T_{\mathrm{incoh}} = \frac{|t_{as}t_{sb}|^2 \exp\left(-2\frac{\omega}{c}K_s d_s\right)}{1-|r_{sa}r_{sb}|^2 \exp\left(-4\frac{\omega}{c}K_s d_s\right)} \cdot \frac{\mathrm{Re}\{\tilde{N}_b/\mu_b\}}{\cos\alpha}. \tag{17}$$

The factor $\mathrm{Re}\{\tilde{N}_b/\mu_b\}/\cos\alpha$ vanishes if medium b is the same as medium a – in our case vacuum. The information about the phase and attenuation of amplitude carried by the exponential function $\phi_s = \exp[i(\omega/c)\tilde{N}_s d_s]$ through the substrate reduces to a pure attenuation of intensity $\exp[-2(\omega/c)K_s d_s]$.
It should be emphasized that complete internal coherence of the films at the front and back of the substrate, survives separately.

2.2. Arbitrary Succession of Films and Substrates

The formalism of multiple reflection can be extended to systems with more than one incoherent plate. As an example, we consider in Fig. 3 a system consisting of 3 piles of thin films and 2 thick plates. First, one has to write down the reflectance and transmittance for one of the two plates according to (16 and 17). In this step the second plate is taken into account together with two piles of films. The contribution of the latter system has to be decomposed again according to (16 and 17). This procedure can be continued for an arbitrary number of plates.
An equivalent method, not showing the close connection to the concept of multiple reflection, consists of splitting the whole transfer matrix $\mathbf{T}$ into parts like (13). To get the desired averaged reflectance and transmittance we have to take the absolute squares like

$$\frac{1}{|t_{ij}|^2}\begin{Bmatrix} 1 & -|r_{ji}|^2 \\ |r_{ij}|^2 & |t_{ij}t_{ji}|^2 - |r_{ij}r_{ji}|^2 \end{Bmatrix}, \tag{18}$$

$$\frac{1}{|\phi_j|^2}\begin{Bmatrix} 1 & 0 \\ 0 & |\phi_j|^4 \end{Bmatrix} \tag{19}$$

and then evaluate the complete matrix product. Thus we get the incoherent transfer matrix $\mathbf{T}_{\mathrm{incoh}}$ and the reflectance

$$R_{\mathrm{incoh}} = T_{21,\mathrm{incoh}}/T_{11,\mathrm{incoh}} \tag{20}$$

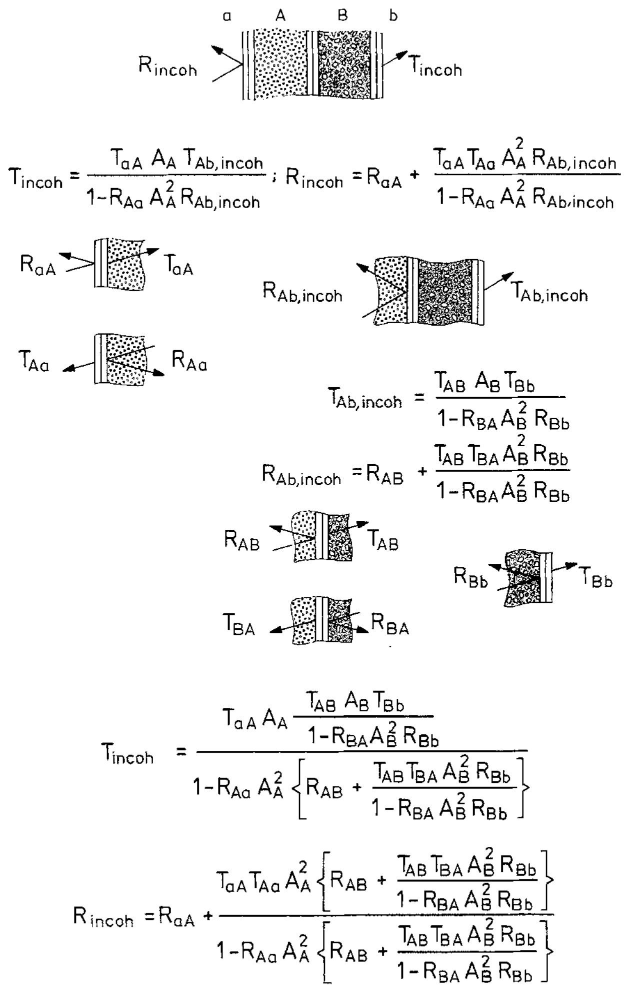

Fig. 3. Strategy to calculate the reflectance and transmittance of films separated by two incoherent substrates as an example for the "concept of multiple reflection". $A_{A,B} = \exp[-(\omega/c)K_{A,B}d_{A,B}]$: attenuation for one path through the substrate A, B

and the transmittance, if medium a and b are equal, e.g. vacuum

$$T_{\mathrm{incoh}} = 1/T_{11,\mathrm{incoh}}. \tag{21}$$

In case of the example of Fig. 3 the procedure leads to the expression shown in Fig. 4.[2]
If there are two substrates joining each other, they are linked by the matrix of their Fresnel coefficients which must be written down in the sense of (18) as

$$\frac{1}{|\tau_{ij}|^2}\begin{Bmatrix} 1 & -|\varrho_{ji}|^2 \\ |\varrho_{ij}|^2 & |\tau_{ij}\tau_{ji}|^2 - |\varrho_{ij}\varrho_{ji}|^2 \end{Bmatrix}. \tag{22}$$

Of course we have $\varrho_{ij} = -\varrho_{ji}$ and $\tau_{ij} = 1 + \varrho_{ij}$.

[2] For example with two substrates this can be proven by explicit calculation. For an arbitrary number of substrates, a proof should use the one-to-one mapping of $\mathbf{T}$ by the r and t.

$$\begin{Bmatrix}1\\ R_{incoh}\end{Bmatrix} = \frac{1}{T_{aA}}\begin{Bmatrix} 1 & -R_{Aa} \\ R_{aA} & T_{aA}T_{Aa}-R_{aA}R_{Aa}\end{Bmatrix}$$

$$\frac{1}{A_A}\begin{Bmatrix}1 & 0\\ 0 & A_A^2\end{Bmatrix}\frac{1}{T_{AB}}\begin{Bmatrix}1 & -R_{BA}\\ R_{AB} & T_{AB}T_{BA}-R_{AB}R_{BA}\end{Bmatrix}$$

$$\frac{1}{A_B}\begin{Bmatrix}1 & 0\\ 0 & A_B^2\end{Bmatrix}\frac{1}{T_{Bb}}\begin{Bmatrix}1 & -R_{bB}\\ R_{Bb} & T_{Bb}T_{bB}-R_{Bb}R_{bB}\end{Bmatrix}\cdot\begin{Bmatrix}T_{incoh}\\ 0\end{Bmatrix}$$

Fig. 4. Reflectance and transmittance of the example of Fig. 3 in the matrix formalism

2.3. Comparison of the Concept of Incoherent Multiple Reflections with the Method of Averaging

A widely used straightforward method suppresses the Fabry-Perot structures of the substrates by numerical averaging. In this method the spectral window of the experiment is simulated: The coherent reflectance and transmittance of the pile is calculated for a high number of sampling points sufficiently close to resolve the interferencies of the substrates. Then, a convolution with the spectral window leads to the desired result [4].

This method of averaging is very time consuming, since one has to compute the reflectance for a very fine mesh of frequencies. Generally, the variation in frequency of all quantities r, t, and ϕ is smooth compared to the "unwanted" Fabry-Perot structures. Therefore the concept of incoherent multiple reflection leads to the same results.[3] Our method, however, drastically reduces the time of computation since reflectance and transmittance have to be calculated at much fewer sampling points. As example, we show the results for the reflectance of a system of two epitactic layers on a substrate in Fig. 5. The difference between the spectra calculated by the two methods cannot be resolved in this plot. The number of necessary points for the method of averaging is larger by a factor of 25 compared to our concept.

[3] To prove this we expand the geometrical series in (15) and take the absolute square of the whole expression. Products like $\phi^m \cdot (\phi^n)^*$ occur. The terms with $m \neq n$ vary sinusoidally with frequency. Consequently, after integration, only terms with $m = n$ survive. Thus, one obtaines the same formulae, as predicted by the concept of incoherent multiple reflection

3. Conclusion

We have presented a method – based on the idea of multiple reflections of field amplitudes – to calculate the reflectance and transmittance of a pile of layers. This method is able to take into account complete coherence of all films as well as incoherent propagation within individual layers. This is important simulating spectra measured at limited resolution or in the presence of other interference destroying effects.

Examples for possible applications are presented in Fig. 6.

Moreover, in the concept of multiple reflection it is possible to calculate up to any desired number of reflections (with or without interference). This may

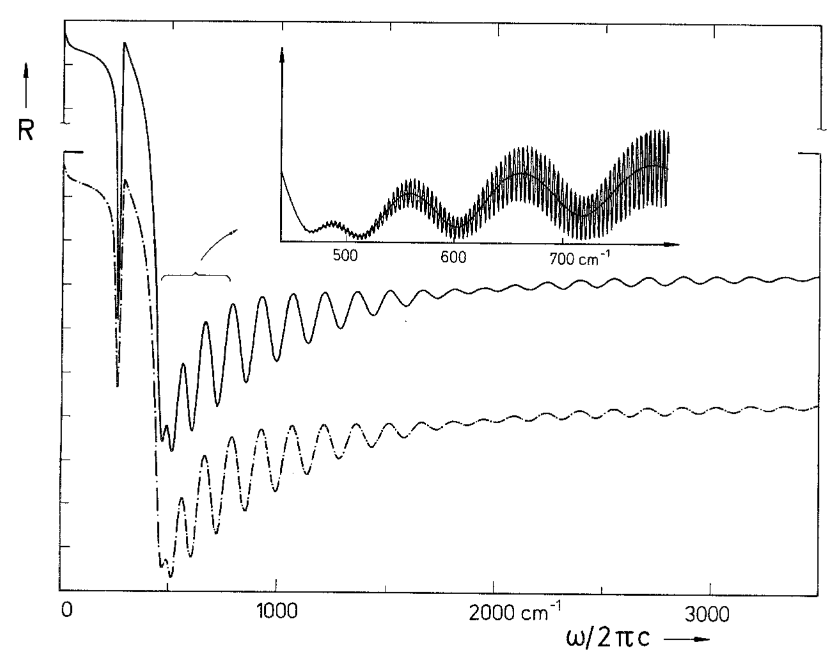

Fig. 5. Calculation of the reflectance of a two layer system deposited on a GaAs substrate ($d = 0.35$ mm) [2]. The two layers consist of an epitaxial grown doped GaAs film ($n = 1.8 \times 10^{18}$ cm^{-3}, $d = 8.8$ μm) and an interfacial layer ($n = 4 \times 10^{18}$ cm^{-3}, $d = 0.8$ μm). The insert shows the rapid oscillations due to the substrate which are not resolved by the measurement. ——— Calculation with the "concept of multiple reflection", --- calculation with the "method of averaging"

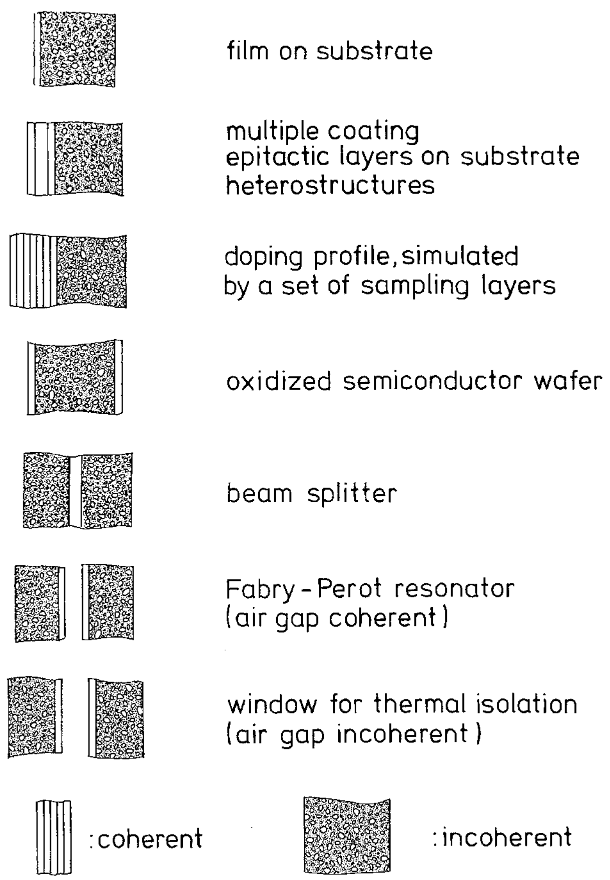

Fig. 6. Examples of applications

become important, e.g., in the case of oblique incidence, in which not all reflected partial waves reach the aperture of the collimator.
We believe, finally, that the representation given above is well adapted to describe the situation in which a layer only shows partial coherence, e.g., due to scattering at a rough surface [5].

Appendix

In the preceeding sections we have developed the formalism explicitly for the case in which the electric field is parallel to the surfaces, i.e. s-polarization.

In case of p-polarization the magnetic field in turn is parallel to the surfaces of the films.
We therefore replace, in the case of p-polarization, the electric fields which occur in the formulae of Sects. 1 and 2 by the magnetic fields:

$$E(z)=E^{(+)}(z)+E^{(-)}(z)\rightarrow H(z)=H^{(+)}(z)+H^{(-)}(z).$$

Instead of (5) the Fresnel coefficients are

$$\varrho_{l,l-1}=\frac{\tilde{N}_l/\varepsilon_l-\tilde{N}_{l-1}/\varepsilon_{l-1}}{\tilde{N}_l/\varepsilon_l+\tilde{N}_{l-1}/\varepsilon_{l-1}}, \quad \tau_{l,l-1}=\frac{2\tilde{N}_l/\varepsilon_l}{\tilde{N}_l/\varepsilon_l+\tilde{N}_{l-1}/\varepsilon_{l-1}}. \tag{23}$$

In addition, we must redefine the coefficients of reflection and transmission (7) in terms of H,

$$r_{ab}\overset{\det}{=}\frac{H_r(z=0)}{H_i(z=0)}, \quad t_{ab}\overset{\det}{=}\frac{H_t(z=z_1)}{H_i(z=0)}. \tag{24}$$

Finally, we have to change the factor $\mathrm{Re}[\tilde{N}_b/\mu_b]/\cos\alpha$ in (17) to $\mathrm{Re}\{\tilde{N}_b/\varepsilon_b\}/\cos\alpha$.

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