reflection phenomenon that occurs at one interface disappear. These interference and tunneling processes can occur for photons, phonons, and electrons. In this section, we will first examine the interference phenomenon. The formulation established can also be applied to tunneling processes, which will be discussed in section 5.4.

5.3.1 Propagation of EM Waves

There are three ways to derive an expression for the radiative properties (reflectivity and transmissivity) of thin films: the field-tracing method, the resultant wave method, and the transfer matrix method, as explained in figure 5.9. The field-tracing method, figure 5.9(a), follows the trajectory of the wave and counts each reflection and transmission when the wave meets an interface (Born and Wolf, 1980), using the Fresnel reflection and transmission coefficients. This method is intuitive but cumbersome. Because all the forwarding waves in the same medium have the same exponential factor, we can sum them up into one wave with a undetermined amplitude and call this wave the resultant wave [figure 5.9(b)]. Similarly, all the backward propagating waves in the same medium can be summed into a resultant wave. There are then four resultant waves in the single layer thin film situation, one reflected, two inside the film (forward and backward), and one transmitted, as shown in figure 5.9(b). The amplitude of each resultant wave will be determined by applying the boundary conditions at the two interfaces. The transfer matrix method combines all the waves (both forward and backward) in each medium into one wave, and uses a matrix to relate the electric and magnetic fields between two different points inside a medium, as shown in figure 5.9(c). Because the tangential components of the electric and magnetic fields are continuous across the interface when no interface charge or interface current exists, the transfer matrix method can be easily extended to multilayers. We will therefore focus on the transfer matrix method.

Consider a TM wave, for example, the x-component of the electric field and the y-component of the magnetic field inside the film, as a function of location z:

$$E_x(z) = \cos\theta_2 E^+ e^{i\varphi(z)} + \cos\theta_2 E^- e^{-i\varphi(z)} \tag{5.102}$$

$$H_y(z) = \frac{n_2}{\mu c_0}[E^+ e^{i\varphi(z)} - E^- e^{i\varphi(z)}] \tag{5.103}$$

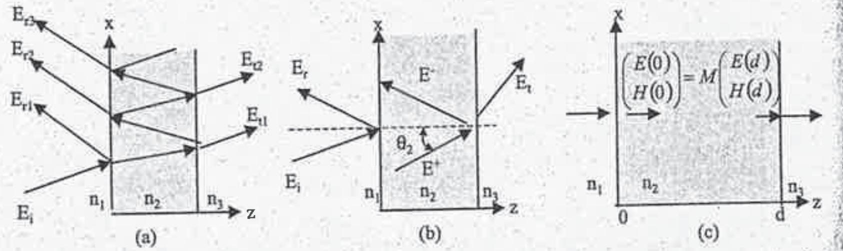

Figure 5.9 Three methods of treating reflection and transmission of electromagnetic fields through a thin film: (a) the field tracing method; (b) the resultant wave method; (c) the transfer matrix method.

where E^+ and E^- are the amplitudes of the resultant forward and backward propagating waves inside the film and

$$\varphi(z) = \frac{\omega n_2 z \cos\theta_2}{c_0} \tag{5.104}$$

where θ_2 is the angle formed between wavevector direction and z. Again, if n_2 is complex, this angle is also complex, and can be calculated according to the Snell law. In the above equations, we have dropped the terms $\exp(-i\omega t)$ and $\exp(-k_x x)$ because all terms have these factors and eventually cancel.

We want to relate the electric and magnetic fields at any location z inside the film to these fields at the interface $z = 0$. This can be realized by first taking $z = 0$ in eq. (5.102) and (5.103) and then eliminating E^+ and E^- in these equations,

$$E_x(z) = E_x(0)\cos\varphi(z) + ip_2 H(0)\sin\varphi(z) \tag{5.105}$$

$$H_y(z) = \frac{i}{p_2}E_x(0)\sin\varphi(z) + H_y(0)\cos\varphi(z) \tag{5.106}$$

where $p_2 = [\cos\theta_2/(n_2/\mu c_o)]$ is the *surface impedance* for a TM wave. The above equations can be written in matrix form

$$\begin{pmatrix}E_x(z)\\H_y(z)\end{pmatrix} = \begin{pmatrix}\cos\varphi(z) & ip_2\sin\varphi(z)\\ \frac{i}{p_2}\sin\varphi(z) & \cos\varphi(z)\end{pmatrix}\begin{pmatrix}E_x(0)\\H_y(0)\end{pmatrix} \tag{5.107}$$

Taking $z = d$ and inverting the above matrix, we get

$$\begin{pmatrix}E_x(0)\\H_x(0)\end{pmatrix} = \begin{pmatrix}\cos\varphi_2 & -ip_2\sin\varphi_2\\ -\frac{i}{p_2}\sin\varphi_2 & \cos\varphi_2\end{pmatrix}\begin{pmatrix}E_x(d)\\H_y(d)\end{pmatrix} = M\begin{pmatrix}E_x(d)\\H_y(d)\end{pmatrix} \tag{5.108}$$

where $\varphi_2 = \varphi(d)$ and M is the second-order matrix in the above equation. We call M the interference matrix. It is easy to show that $|M| = 1$.

Equation (5.108) relates the electric and magnetic fields inside the film at $z = d$ to their values at the boundary $z = 0$. To find the reflectivity or transmissivity, we need to further relate them to the fields outside the film through the boundary conditions. For a boundary free of charge and current, eqs. (5.58) and (5.61) dictate that the electric and magnetic fields are continuous, which means that at $z = 0$,

$$E_x(0) = E_i\cos\theta_i + E_r\cos\theta_r = E_{ix} + E_{rx} \tag{5.109}$$

$$H_y(0) = \frac{n_1}{\mu c_0}(E_i - E_r) = \frac{1}{p_1}(E_{ix} - E_{rx}) \tag{5.110}$$

and at $z = d$, only the transmitted wave exists,

$$E_x(d) = E_t\cos\theta_t = E_{tx} \tag{5.111}$$

$$H_y(d) = \frac{n_3}{\mu c_0}E_t = \frac{1}{p_3}E_{tx} \tag{5.112}$$

where $p_1 = \cos\theta_i/(n_1/\mu c_0)$ and $p_3 = \cos\theta_t/(n_3/\mu c_0)$, and we have assumed that μ is the same for all layers because most materials are diamagnetic in the infrared to visible frequency range. We can again write the above equations in matrix form,

$$\begin{pmatrix} E_x(0) \\ H_y(0) \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ \frac{1}{p_1} & -\frac{1}{p_1} \end{pmatrix} \begin{pmatrix} E_{ix} \\ E_{rx} \end{pmatrix} \tag{5.113}$$

$$\begin{pmatrix} E_x(d) \\ H_y(d) \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{p_3} \end{pmatrix} E_{tx} \tag{5.114}$$

We now combine eqs. (5.113), (5.114), and (5.108), using the continuity of E_x and H_y at the interfaces, to get

$$\begin{pmatrix} 1 & 1 \\ \frac{1}{p_1} & -\frac{1}{p_1} \end{pmatrix} \begin{pmatrix} E_{ix} \\ E_{rx} \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1}{p_3} \end{pmatrix} E_{tx} \tag{5.115}$$

where m_{ij} are the elements of the *interference matrix* M. Inverting the matrix of the left-hand side and multiplying out the three matrices, we obtain

$$\begin{pmatrix} E_{ix} \\ E_{rx} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} (m_{11} + \frac{1}{p_3} m_{12}) + (m_{21} + \frac{1}{p_3} m_{22}) p_1 \\ (m_{11} + \frac{1}{p_3} m_{12}) - (m_{21} + \frac{1}{p_3} m_{22}) p_1 \end{pmatrix} E_{tx} \tag{5.116}$$

From the above matrix, we get the reflection and transmission coefficients through the film as

$$r = \frac{E_r}{E_i} = \frac{E_{rx}}{E_{ix}} = \frac{(m_{11} + \frac{1}{p_3} m_{12}) - (m_{21} + \frac{1}{p_3} m_{22}) p_1}{(m_{11} + \frac{1}{p_3} m_{12}) + (m_{21} + \frac{1}{p_3} m_{22}) p_1} \tag{5.117}$$

and

$$t = \frac{E_t}{E_i} = \frac{E_{ix}/\cos\theta_t}{E_{ix}/\cos\theta_i} = \frac{2c_{tm}}{(m_{11} + \frac{1}{p_3} m_{12}) + (m_{21} + \frac{1}{p_3} m_{22}) p_1} \tag{5.118}$$

where $c_{tm} = \cos\theta_i/\cos\theta_t$. For a TE wave, the above expressions are still valid if p and c_{tm} are replaced by

$$p = -\frac{n\cos\theta}{\mu c_0} \text{ and } c_{te} = 1 \tag{5.119}$$

With the reflection and transmission coefficients known, we can calculate the reflectivity and transmissivity according to eqs. (5.75) and (5.76). For absorbing films, the above formulation is still valid by if n is replaced with the complex refractive index N.

The power of the matrix method can be best appreciated when dealing with multilayers of thin films. In this case, we can relate the electric and magnetic field inside the ith layer at both interfaces by the interference matrix M_i for that layer. Since the transverse components of the electric and magnetic fields are continuous at each interface that is free of net charge and current, the total interference matrix of the whole multilayer structure is

$$M = M_1 M_2 M_3 \ldots M_n \tag{5.120}$$

Thus, with such a simple substitution, all previous expressions for the single-layer film are still valid.

For a single layer of film, eqs. (5.117) and (5.118) can be written as

$$r = \frac{r_{12} + r_{23}e^{2i\varphi_2}}{1 + r_{12}r_{23}e^{2i\varphi_2}} \tag{5.121}$$

and

$$t = \frac{t_{12}t_{23}e^{i\varphi_2}}{1 + r_{12}r_{23}e^{2i\varphi_2}} \tag{5.122}$$

where r_{12}, r_{23} and t_{12}, t_{23} are the Fresnel reflection and transmission coefficients from medium 1 into medium 2 or from medium 2 to medium 3. The above formula is valid for both TM and TE waves.

On the basis of these expressions, we can calculate the reflectivity and transmissivity of the film. For a nonabsorbing film,

$$R = |r|^2 = \frac{r_{12}^2 + r_{23}^2 + 2r_{12}r_{23}\cos 2\varphi_2}{1 + 2r_{12}r_{23}\cos 2\varphi_2 + r_{12}^2 r_{23}^2} \tag{5.123}$$

$$\tau = \frac{n_3\cos\theta_t}{n_1\cos\theta_i}|t|^2 = \frac{(1 - r_{12}^2)(1 - r_{23}^2)}{1 + 2r_{12}r_{23}\cos 2\varphi_2 + r_{12}^2 r_{23}^2} \tag{5.124}$$

If the optical constants of any media are complex, we should use eq. (5.76) to calculate the transmissivity, and carry out complex number operation, $R = rr^*$ and $\tau = tt^*$.

The cosine function in eqs. (5.123) and (5.124) suggests that the reflectivity and transmissivity vary as a function of thickness, and when there is no absorption the variation is periodic, as shown in figure 5.10. This periodic variation in reflectivity and

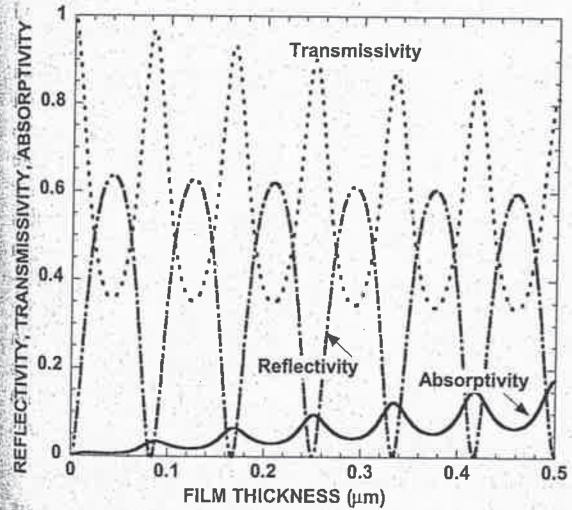

Figure 5.10 Reflectivity, transmissivity, and absorptivity of a thin film as a function of the film thickness, assuming vacuum on both sides.

transmissivity is the *interference phenomenon*, caused by the constructive or destructive superposition of the reflected and the incident waves. The maximum or minimum in the reflectivity can be found by setting $dR/d\varphi_2 = 0$, which leads to

$$\sin 2\varphi_2 = 0 \tag{5.125}$$

or

$$\frac{4\pi n_2 L \cos\theta_2}{\lambda_0} = m\pi \tag{5.126}$$

$$d = \frac{m\lambda_0}{4n_2\cos\theta_2} \tag{5.127}$$

Under the above condition, eq. (5.123) becomes

$$R = \left(\frac{r_{12} - r_{23}}{1 - r_{12}r_{23}}\right)^2 = \left(\frac{n_1 n_3 - n_2^2}{n_1 n_3 + n_2^2}\right)^2 \quad (\text{for odd m} = 2l + 1) \tag{5.128}$$

$$R = \left(\frac{r_{12} + r_{23}}{1 + r_{12}r_{23}}\right)^2 = \left(\frac{n_1 - n_3}{n_1 + n_3}\right)^2 \quad (\text{for even } m = 2l) \tag{5.129}$$

where the first equality in the above two equations is valid for an arbitrary angle of incidence while the second is for normal incidence only. When the film thickness is $(2\ell + 1)\,\lambda_0/(4n_2\cos\theta_2)$, the reflectivity R can be a maximum ($n_2 < n_3$) or a minimum ($n_2 < n_3$). Zero reflection occurs when the film has a refractive index $\sqrt{n_1 n_3}$ and its thickness satisfies eq. (5.127) for odd m. Such interference phenomena are the basis for *antireflection coatings*. When the film thickness is $\ell\lambda_0/(2n_2\cos\theta_2)$, the reflectivity does not depend on the second layer.

The reflectivity and transmissivity of multilayer thin films can be calculated using the transfer matrix method. In practice, the reflectivity and transmissivity of multilayers can be controlled quite accurately with various thin-film deposition techniques and the possibility of controlling spectral and directional properties is large. One special example is the *Bragg reflector*, which is made from two alternating layers of thin films, figure 5.11(a). Each layer has a thickness equal to one-quarter of the light wavelength inside the film. Although, at one interface, the reflectivity between the two materials may be small, the coherent superposition of the reflected fields can create a reflectivity that is close to 100%. Such Bragg reflectors are used as coatings for mirrors that are highly reflective at a specific required wavelength, such as for lasers and X-rays. Figure 5.11(b) gives an example of the reflectivity of a quarter-wavelength mirror, similar to those used in special semiconductor laser structures called vertical-cavity surface-emitting lasers (Koyama et al., 1989; Walker, 1993). The reflectivity in certain spectral regions can reach 100%, meaning that no electromagnetic fields in that wavelength regime exist inside the reflector. These spectral regions, called stop bands, occur when the round-trip phase difference through one period (two layers) equals $2\ell\pi$, that is, when the forward and backward propagating fields inside the films cancel each other,

$$\frac{4\pi n_1 d_1\cos\theta_1}{\lambda_0} + \frac{4\pi n_2 d_2\cos\theta_2}{\lambda_0} = 2\ell\pi \tag{5.130}$$

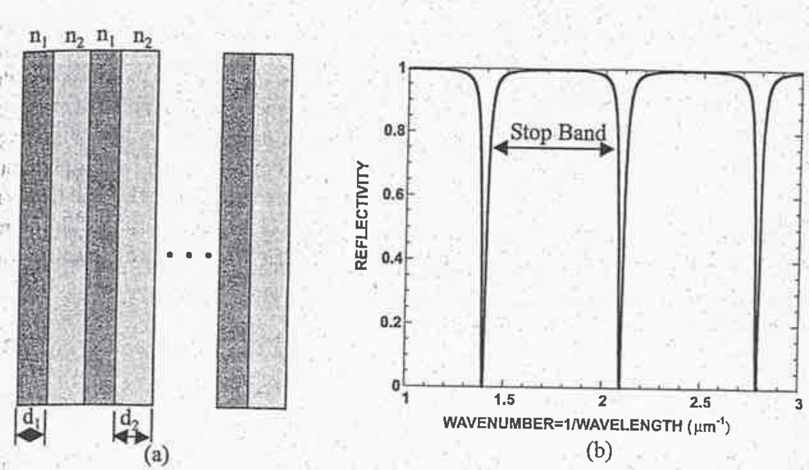

Figure 5.11 (a) A Bragg reflector is a periodic thin-film structure. (b) Calculated reflectivity of a Bragg reflector as a function of the incident photon wavelength for a reflector with refractive indices of 3 and 3.5 and a corresponding thickness of 417 Å and 352 Å for each layer.

where the subscripts 1 and 2 denote layer 1 and layer 2 respectively. Denoting $a = n_1 d_1\cos\theta_1 + n_2 d_2\cos\theta_2$ as the optical thickness of one period, the above equation can be written as (Knittl, 1976)

$$ka = \ell\pi \tag{5.131}$$

where $k(= 2\pi/\lambda_0)$ is the wavevector in vacuum. Equation (5.131) is identical to the condition of the electron bandgap formation discussed in chapter 3, which was obtained by solving the Schrödinger equation. We have said before that the formation of the electron bandgap is due to the cancellation of the electron waves inside the crystal. The discussion on the photon stop bands reinforces this picture. The similarities of these different waves, including electrons, photons, and phonons, have, in the past, been explored extensively to develop new concepts. For example, the *phonon interference filters* (Narayanamurti et al., 1979) and the electron minigaps (Esaki and Tsu, 1970), based on superlattices, benefited from the analogy of photon stop bands in interference filters. In return, it was exactly on the basis of the analogy of three-dimensional band structure in naturally existing crystals for electrons and phonons that the concept of three-dimensional *photonic crystals* was proposed (Yablonovitch, 1986), although one can also argue that this concept is an extension of the thin-film Bragg reflectors to three dimensions. Not only are these concepts very similar to each other; the mathematical techniques are also often interchangeable. For example, one popular approach for calculating the band structures of three-dimensional photonic crystals is based on a generalized transfer matrix method (Pendry, 1996).

5.3.2 Phonons and Acoustic Waves

In chapter 3, we considered phonon waves in a periodic lattice chain and discussed phonons in superlattices. The periodicity in naturally existing crystal lattices leads to the representation of phonons in the first Brillouin zone. The periodicity of superlattices adds an additional restriction to the phonon wavevector and leads to the folded zone representation and the formation of phonon minibands [figure 3.30]. Similar to the photon stop bands, the phonon minigaps formed in the dispersion of superlattices can be thought of as stop bands generated by multiple reflections and coherent superposition of the lattice waves, as for photons in periodic structures. For long-wavelength phonons, that is, acoustic waves, one can also use the transfer matrix method as for optical waves to calculate the transmission of lattice waves through single-layer and multilayer structures (Nayfeh, 1995). The reflectivity r and transmissivity t of an SH wave through a film with thickness d can be calculated from the following matrix

$$\begin{pmatrix} 1 \\ r \end{pmatrix} = A_i^{-1} M A_t \begin{pmatrix} t \\ 0 \end{pmatrix} \tag{5.132}$$

where the interference matrix is similar to that of an electromagnetic wave

$$M = \begin{pmatrix} \cos\varphi_{T2} & i\sin\varphi_{T2}/Y_2 \\ iY_2\sin\varphi_{T2} & \cos\varphi_{T2} \end{pmatrix} \tag{5.133}$$

$$A_i = \begin{pmatrix} 1 & 1 \\ -Z_{Ti}\cos\theta_{Ti} & Z_{Ti}\cos\theta_{Ti} \end{pmatrix} \tag{5.134}$$

where $\varphi_{T2} = \omega d\cos\theta_2/v_{T2}$, $Y_2 = -Z_{T2}\cos\theta_2$, and A_t is obtained by replacing the subscript i in eq. (5.134) by t. The subscript T is used to represent properties of the transverse waves and, in this case, a transverse wave polarized perpendicular to the plane of incidence. The reflection and transmission coefficients are defined as

$$r = v_r(0)/v_i(0) \quad t = v_t(d)/v_i(0) \tag{5.135}$$

The matrix formulation for SH acoustic waves is clearly similar to that for optical waves. Multilayers can again be treated by simply replacing the interference matrix M with the product $M_1M_2\ldots M_{2n+1}$. The order of the matrices is the same as the sequence of the layers. For longitudinal waves (L) and vertically polarized transverse waves (SV) with the displacement polarized in the plane of incidence, the relationship between the incident, reflected, and transmitted wave velocity components of isotropic media is

$$\begin{pmatrix} v_{Ti}(0) \\ v_{Li}(0) \\ v_{Tr}(0) \\ v_{Lr}(0) \end{pmatrix} = B_i^{-1} M B_t \begin{pmatrix} v_{Tt}(d) \\ v_{Lt}(d) \\ 0 \\ 0 \end{pmatrix} \tag{5.136}$$

where v_{Ti} and v_{Li} are the amplitudes of the displacement velocities of the incident transverse and longitudinal waves, respectively, and subscripts r and t represent the reflected and transmitted waves, as usual. Matrix B_i is a 4×4 matrix given by

$$B_i = \begin{pmatrix} -\sin\theta_{Ti} & \cos\theta_{Li} & \sin\theta_{Ti} & -\cos\theta_{Li} \\ \cos\theta_{Ti} & \sin\theta_{Li} & \cos\theta_{Ti} & \sin\theta_{Li} \\ -\mu_1 k_{Ti}\sin 2\theta_{Ti} & (\lambda_1 + 2\mu_1\cos^2\theta_{Li})k_{Li} & -\mu_1 k_{Ti}\sin 2\theta_{Ti} & (\lambda_1 + 2\mu_1\cos^2\theta_{Li})k_{Li} \\ \mu_1 k_{Ti}\cos 2\theta_{Ti} & \mu_1 k_{Li}\sin 2\theta_{Li} & -\mu_1 k_{Ti}\cos 2\theta_{Ti} & -\mu_1 k_{Li}\sin 2\theta_{Li} \end{pmatrix} \tag{5.137}$$

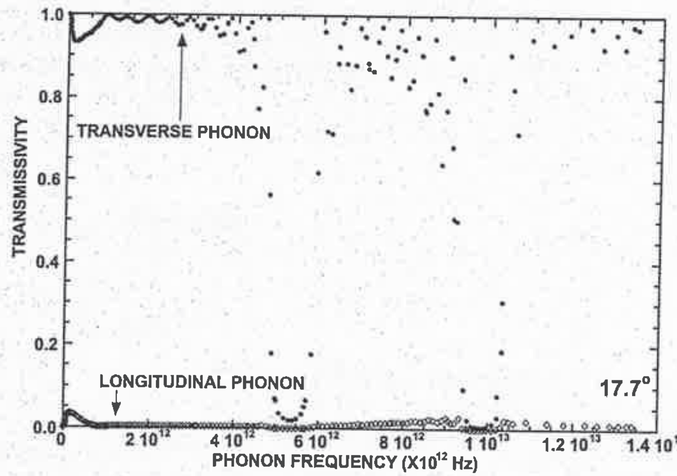

Figure 5.12 Transmissivity of a transverse acoustic wave polarized in the plane of incidence through a Si/Ge-like superlattice as a function of frequency with an incident angle of 17.7° (Chen, 1999).

In the above expressions, $k_i (= \omega/v_i)$ is the magnitude of the wavevector of the incident waves (SV or L, as distinguished by subscripts T and L). B_t is obtained by replacing subscript i with t, that is, from incident to transmitted waves. The interference matrix of the layer (with index 2) in eq. (5.136) is obtained from $M = B_2^{-1}N_2B_2$, where B_2 is obtained by replacing i in eq. (5.137) by 2, and N_2 is given by

$$N_2 = \begin{pmatrix} e^{i\varphi_{T2}} & 0 & 0 & 0 \\ 0 & e^{i\varphi_{L2}} & 0 & 0 \\ 0 & 0 & e^{-i\varphi_{T2}} & 0 \\ 0 & 0 & 0 & e^{-i\varphi_{L2}} \end{pmatrix} \tag{5.138}$$

The transfer matrix is 4×4 because, as shown in eq. (5.136), the longitudinal and transverse waves are coupled and the conversion between these two waves is possible at the interface. With eq. (5.136), the reflectivity and transmissivity for an incident field (either v_{Ti} or v_{Li}) can be calculated.

Figure 5.12 shows an example of phonon transmissivity through a Si/Ge-like superlattice obtained by the transfer matrix method (Chen, 1999), for a transverse wave polarized in the plane of incidence at an angle of incidence of 17.7°. The stop bands in transmissivity (zero transmissivity) correspond to the minigaps obtained from lattice dynamics simulation (figure 3.30) (Yang and Chen, 2001). The figure also shows that some transverse incident waves are converted into longitudinal waves.

5.3.3 Electron Waves

The study of electron wave propagation in layered media started with the investigation on superlattices (Esaki and Tsu, 1970). The most popular approach has been based on