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Energy dependence of the effective mass in the envelope-function approximation

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Abstract

Results of a study on the tunneling electron effective mass as a function of energy and barrier width are reported. A system with a highly selective transmission factor, a double barrier, has been chosen in order to be able to define a particular energy. As the energies of the resonant transmission peaks are mostly determined by the effective mass of the material forming the well, while the transmission-peak width mostly depends on the barrier effective mass, both masses are obtained separately by fitting results for transmission using layers of periodic lattices and using the simplification allowed by the effective-mass approximation. The central well width has been varied and several transmission maxima have been considered, thus covering a wide energy range. The effective-mass in the relatively large barrier is shown to be much lower than the bulk-conduction-band value. For very thin barriers, when the decay length of tunneling electrons becomes of the same order as the barrier width, an anomalous increase in the effective mass is observed for high energies. Finally, we obtain the behavior of the effective mass as a function of energy in a one-dimensional triangular potential profile. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

Due to their simplicity and usefulness in the solution of practical problems, the envelope function method and the effective-mass approximation have been widely used together in the study of heterostructures. Although the effective-mass approximation has been theoretically justified only in

the bulk of wide systems [1], it has been used even in multilayered systems in which very narrow layers are present. To assume that properties corresponding to an infinite bulk material can be used for a very thin layer of this material when it forms a barrier between layers of different materials is highly questionable. Nevertheless, the lack of detailed information about the crystal potential and the formidable task involved in using it in three-dimensional simulations with spatially variable electric fields have made the effective-mass approximation very common in electron device analysis even with very narrow layers. Furthermore,

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numerous examples can be found in the literature in which the effective-mass approximation is claimed to produce good results, provided that suitable values are chosen. Notably, transmission through a single barrier of AlAs 1.42 nm thick, placed between two GaAs layers [2], which can be regarded as very narrow since the AlAs lattice constant is 0.57 nm. Even in narrow barriers of amorphous materials like SiO₂ the effective-mass approximation has been reported to produce good results with a barrier thickness of 1.4 nm [3]. Transmission through AlAs barriers with a very small thickness (1.05 nm) in a GaAs/AlAs superlattice was reported by Brozak et al. [4], where a renormalized effective mass was used. In general, as the envelope-function approximation produces good results, its validity is assumed in each layer of the heterostructure. Therefore, the remaining problem is to choose suitable boundary conditions. Detailed studies have been performed on precisely this issue [5,6].

Notwithstanding, even if the validity of the envelope-function approximation is assumed, a remaining question is the appropriate effective-mass value that should be chosen for each layer. The mass corresponding to the minimum of the conduction band is usually used when dealing with electron transport. However, this choice can be questioned in several specific cases. For example, in a quantum well the allowed energy levels are well above the conduction band minimum of the well material. Non-parabolicity effects are therefore important [7] and the effective mass must be modified. The use of the conduction-band minimum mass is even more questionable when considering transmission through a barrier, since tunneling usually takes place at an energy well below the barrier conduction-band edge. In this case there are no physical reasons to assign a conduction-band mass to an energy level inside the band gap of the barrier material and so the use of the band edge barrier effective mass is extremely suspect and the real band structures of the barrier should be taken into consideration. It would be more reasonable to use a dispersion relationship with participation of both the conduction- and valence-band effective masses. But as the effective mass of electrons at the top of the valence band is negative, the effective mass inside the band gap should decrease with energy,

even changing its sign at an energy value close to the middle of the band gap, where a zero value can be accepted. This result has been reported by Ando and Akera [8]. A similar result was obtained by Bowen et al. [9], who showed that a parabolic $E-k$ dispersion relationship in the barriers cannot accurately reproduce experimental current-voltage curves in a double-barrier diode, while much better agreement with experimental results is obtained if the $E-k$ dispersion calculated with a ten-band model is used. Nevertheless, another possibility is that the effective mass of electrons which cross a narrow barrier is influenced by the materials on both sides of the barrier in addition to the influence of the barrier material itself, as concluded by Brozak et al. [4]. Considering only parameters for the barrier material, in computing the energy-dependent effective mass within it, may be therefore insufficient, it being important to consider properties of the material on both sides of the barrier as well.

An additional question is the lowest barrier thickness at which the effective-mass approximation, even with an energy dependence, can produce accurate results. Of course the concept of effective mass makes no sense in barriers with only one lattice period. But even with several lattice periods the effective-mass concept in the barrier should only be used at energies at which the barrier thickness is several times higher than the inverse of the damping factor. Given these difficulties in choosing the effective-mass value, the aim of this paper has been to test the effective-mass approximation as a function of energy as well as of the barrier width. To select a definite energy, a system with a highly selective transmission factor has been chosen: a double barrier. As it is well known, transmission peaks are obtained at energies very close to the central well levels. Their energies are therefore determined by the well material effective mass. On the other hand, disregarding scattering-assisted transitions, the transmission-peak width is determined by the transmission of the two barriers [10] and is thus dependent on the barrier effective mass. As a consequence, if the energy position and width of a transmission peak obtained in a 'real' double barrier are compared to the energy position and width of the transmission peak obtained with the effective-mass approximation, information

concerning the well and barrier effective masses can be gathered at the energy of the transmission maximum. By varying the central well width and considering several transmission maxima, this study can be accomplished across a wide energy range, which is the procedure used in this paper.

One of the main objectives of this paper is a qualitative description of the expected properties of the effective masses for both the well material and the barrier material in a heterostructure. To perform this qualitative study, we need to solve exactly a model in which the periodic potential at atomic scale is taken into account (from now on, we will term it as a ‘real’ crystal), and we have to compare these exact results with the ones obtained from the envelope function method in the effective-mass approximation, that disregards the periodicity of the potential at atomic scale. Our choice for the exactly solvable model is a ‘real’ binary lattice in which the periodic potential is represented by a Kronig–Penney series of δ functions. The transmission through this system has been calculated and an attempt has been made to reproduce it with the simpler potential provided by the effective-mass approximation. The effective masses of the materials of the well and of the barrier have been modified to achieve good agreement both in the position and width of the transmission peaks. In previous works, results given by Kronig–Penney lattices have been compared with those produced by the envelope-function approximation in a single heterojunction, allowing the analysis of matching conditions in one heterointerface [11]. Nevertheless, with the procedure used here, the mass in the two materials, well and barrier, can be studied *separately*. Following sections present the calculation procedure, a more detailed description of the system, and also our most significant results.

2. Method of calculation

In order to calculate the transmission coefficient through the double barrier in both cases, in the ‘real’ crystal and in the envelope-function approximation, we used the characteristic determinant method, which is closely related to the Green function (GF) of the whole system [12,13]. This method

can be considered as an alternative to the widely used transfer matrix method and provides not only the transmission coefficient of the system, but also the density of states and, if the system is closed, its bound states. This method has been shown to be very valuable in the study of random [12] as well as quasiperiodic [14] one-dimensional systems, even in the presence of applied electric and magnetic fields [15,16].

The double-barrier heterostructure is built in both cases by using a multilayered system. In the structure we termed ‘real crystal’, we consider the case where the extent of each individual potential $V(x)$ is small as compared to any other typical length of the system. In particular, the different layers are pieces of Kronig–Penney lattices built with δ -function barriers. Note, however, that generally this simplification with Kronig–Penney lattices is not necessary for applying the method discussed here. As for the envelope-function approximation, the layers are just homogeneous pieces characterized by their lengths and the constant value of their potential energy.

For such multilayered systems, the method of the characteristic determinant presents some features that greatly facilitate the numerical calculation. The basic idea of the method is to take into account multiple interfaces consistently and exactly without making use of the perturbation theory (see Ref. [13] for more details). In this method the Green function (GF) is first evaluated when one boundary between two media is available. In the case of two boundaries, the problem is solved using the GF for one boundary. Therefore we can solve the problem iteratively with $n + 1$ boundaries, considering the solution with n boundaries to be known. In the case of two semi-infinite media A and B we have the conditions of the GF continuity and the equality of currents at the boundary $x = x_1$:

$$G_A(x_1, x_1) = G_B(x_1, x_1),$$

$$\frac{\partial}{\partial x_1} G_A(x_1, x_1) = \frac{\partial}{\partial x_1} G_B(x_1, x_1), \quad (1)$$

where $G_A(x, x)$ ($G_B(x, x)$) are the *exact* one-dimensional GF to the left (right) of boundary x_1 . The initial information needed to apply the method is just the exact GF $G_i(x, x)$ ($i = 1, 2, \dots, N$) of each

one of the N layers of the system, but when these layers are considered to be isolated and infinite materials.

The next step for the further calculation is to determine the appropriate boundary conditions at abrupt interfaces in the frame of the effective-mass theory. We restrict ourselves to only the most widely used boundary conditions (see Ref. [6] for more details),

$$\begin{aligned} \tilde{G}_A(x_1, x_1) &= \tilde{G}_B(x_1, x_1), \\ \frac{1}{m_A^*} \frac{\partial}{\partial x_1} \tilde{G}_A(x_1, x_1) &= \frac{1}{m_B^*} \frac{\partial}{\partial x_1} \tilde{G}_B(x_1, x_1), \end{aligned} \quad (2)$$

where $m_{A,B}^*$ is the electron effective mass in the corresponding region. Note that we have written in the previous equation $\tilde{G}_{A(B)}$ instead of $G_{A(B)}$. The symbol ‘ $\tilde{\sim}$ ’ indicates that the GF are not exact, in the sense that they are written in terms of the effective masses, that is the approximation usually considered. Further calculations indicate that the final results, concerning the calculations of the transmission coefficient of the heterostructure, the density of states, etc., remain unchanged when the matching (1) for the exact GF are replaced by conditions (2) valid for the GF written in terms of the effective mass (see, Ref. [17] for more details). With these boundary conditions, we can use the characteristic determinant by the substitution of the exact GF by the GF in the effective-mass approximation.

In the cases we are studying, the determinant, in general a complex function of energy E , satisfies the following recurrence relationship:

$$D_i = A_i D_{i-1} - B_i D_{i-2}, \quad (3)$$

where the explicit dependence on energy E has been omitted and index i ranges from 1 to N , where N is the total number of layers. The initial conditions are

$$D_{-1} = 0; \quad D_0 = 1; \quad A_1 = 1. \quad (4)$$

The values of A_i and B_i are given by ($i > 1$)

$$A_i = 1 + \lambda_{i-1,i} \frac{r_{i-1,i}}{r_{i-2,i-1}} (1 - r_{i-2,i-1} - r_{i-1,i-2}) \quad (5)$$

and

$$B_i = \lambda_{i-1,i} \frac{r_{i-1,i}}{r_{i-2,i-1}} (1 - r_{i-2,i-1})(1 - r_{i-1,i-2}), \quad (6)$$

where $r_{i-1,i}$ is the reflection amplitude between layers $i - 1$ and i , in general given by

$$r_{i-1,i} = \frac{G_{i-1} - G_i}{G_{i-1} + G_i}. \quad (7)$$

$G_i \equiv G_i(x, x)$ is the GF of the same coordinates in layer i -th. The last magnitudes involved in the calculation of the characteristic determinant are functions $\lambda_{i-1,i}$, defined as

$$\lambda_{i-1,i} = \exp\left(\int_{x_{i-1}}^{x_i} dx \frac{1}{2G_i}\right),$$

where x_{i-1} and x_i are the boundaries of layer $i - 1$. As mentioned above, all the magnitudes needed to calculate the characteristic determinant can be obtained if the N Green functions G_i are known. Moreover, this fact makes this method exceptionally general, since the layers can be of totally different materials, and their properties are introduced in the total system by their GF.

To obtain the transmission coefficient of the whole system, it is necessary to define an auxiliary determinant from D_N , termed D_N^1 , with the expression

$$D_N^1 = D_N \left(\lambda_{1,N} \prod_{i=1}^N (1 - r_{i,i-1})(1 - r_{i-1,i}) \right)^{-1/2}. \quad (8)$$

The transmission coefficient is finally obtained from the compact expression

$$T_N = |D_N^1|^{-2}. \quad (9)$$

3. Construction of the system

3.1. Double-barrier heterostructure

We built a one-dimensional double-barrier heterostructure formed by two different binary crystals, each consisting of a piece of a Kronig–Penney (KP) lattice made of δ -function potentials [11]. We designed two different crystals, A and B, and formed the structure ABABA. By using an

appropriate choice of δ -function amplitudes in the A and B materials, named V_A and V_B , respectively, we obtained a double-barrier heterostructure.

To apply the method set forth in the previous section in this system, we needed to know the exact Green function $G_n(x, x)$ ($n = A, B$) of an infinite Kronig–Penney crystal, made of δ -function potentials. The result for an energy E inside an allowed band is given by (see e.g. Ref. [18])

$$G_n(x, x) = \frac{i|\sin ka|}{2k \sin \beta_n a} \left\{ 1 + \frac{V_n \sin kx \sin k(a-x)}{k \sin ka} \right\}, \quad (10)$$

where V_n is the amplitude of the δ barriers that form the crystal, a is the lattice constant, which is the same for both lattices, $k = \sqrt{E}$ (we consider from now on that $\hbar = 2m_0 = 1$, where m_0 is the free electron mass), and β_n plays the role of quasimomentum and its relationship with energy E is given by the standard KP dispersion relation

$$\cos \beta_n a = \cos ka + \frac{V_n}{2k} \sin ka. \quad (11)$$

When the modulus of the RHS in Eq. (11) turns out to be greater than 1, β_n has to be taken as imaginary ($\beta_n = i\gamma_n, \gamma_n > 0$). This situation corresponds to a forbidden energy gap.

It is important to point out that the use of GF of the type (10) (which is a Bloch Green function) implies that the δ -crystal A at both sides of the sequence ABABA is infinite, and therefore corresponds to bulk material of type A.

In the case of the envelope function approximation, we used two layers, A and B, of constant potential energy E_A and E_B , and arranged the sequence ABABA. The values of E_A and E_B were chosen such that the difference $E_B - E_A$, which is the height of the two barriers, is equal to the difference of the energy-band minima in the ‘real’ structure. Without loss of generality, E_A can be set to zero. We obtained the barrier height from the energy difference between the conduction-band minima in A and B, and the effective masses from fitting curvatures at the band edges.

In order to obtain the effective mass of the ‘real’ crystal as a function of energy, we compared the transmission coefficient of the heterostructure

formed with δ -function crystals to the transmission coefficient in the envelope-function approximation, both calculated from the characteristic determinant. In the effective-mass approximation the unperturbed GF in the materials A, B can be written in the standard form

$$\tilde{G}_{A,B}(x, x) = \frac{im_{A,B}^*}{\sqrt{2m_{A,B}^*(E - E_{A,B})}}. \quad (12)$$

The method used to obtain the value of the effective mass makes use of the resonant peaks of the double barrier. By means of an iterative procedure, we consecutively varied the values of m_A^* and m_B^* to fit not only the position of the first resonant peak on the energy axis, but also its width. An example of this type of fit is shown in Fig. 1, where the transmission coefficient of the real double barrier around a resonant peak (solid line) and the fitted transmission coefficient in the envelope-function approximation (dashed line) are represented. The perfect adjustment obtained allowed us to determine the values of the two effective masses at the energy of the resonant peak. Once the resonant

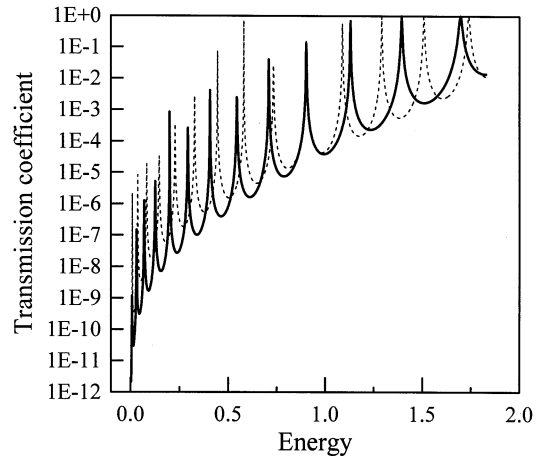


Fig. 1. Plot of an example of the fitting method used in the paper. The solid line represents the transmission coefficient of the real heterostructure, and the dotted line corresponds to the same magnitude using the envelope-function approximation. We fit not only the position of the resonance (mainly controlled by m_A^*), but also its width (mainly controlled by m_B^*). This allows us to determine the two masses for the energy of the resonance.

peak of the real heterostructure has been matched properly, as just described, separate values of m_A^* and m_B^* are determined for this energy. Nevertheless, it is worth noting that this good agreement is obtained only for one peak, corresponding to the energy being considered.

3.2. Abrupt heterostructure in an electric field

In order to discuss the behavior of the effective mass in an external electric field and complete our calculations, we have used a method similar to that detailed in the previous subsection. This can be considered not only as a separate case but also as an application of the results obtained with the method in that subsection. This barrier corresponds to the sequence AB, but with an electric field applied in material B. The scheme of potential energy is shown in Fig. 2.

In the real crystal the continuous linear decrease of the potential in material B is replaced by closely spaced potential steps. Each step consists of two atomic layers within which the potential is constant. The energy difference between consecutive steps is made compatible with the strength of the

applied field by appropriately changing the lowest value of k within the steps in Eq. (10). The corresponding k_i for layer i will be given by

$$k_i = \sqrt{E + L(i - 1) \times eF}, \tag{13}$$

where F is the modulus of the homogeneous applied electric field, e is the electron charge and L is the length of layer i . The term $(i - 1)$ is included since for layer $i = 1$ (the first small piece of material B), the origin of energy remains unchanged, and therefore the barrier in this position has the same height as in the $F = 0$ case.

In the envelope-function approximation, we built the same structure as in the real crystal, formed by layers of constant potential energy with decreasing value in the direction of the field. We used the same length for each layer as in the real crystal, characterizing them by their effective masses. As the potential is constant in each small layer, the boundary conditions (2) also remain valid.

4. Results and discussion

4.1. Double barrier

The result for the effective mass in the A material, m_A^* , obtained using the methods described earlier, is shown in Fig. 3 as a function of energy. The effective masses right in the conduction-band minima for the A and B infinite lattices, m_1 and m_2 , respectively, are plotted in solid circles, with the smallest value corresponding to the A lattice. A monotonic increasing behavior of m_A^* with energy can be observed. The energy ranges from E_A to E_B , which is the height of the barrier.

The curves in Fig. 4 show in symbols the dependence of the effective mass m_B^* in the barrier (material B) on the energy, for different values of the barrier width (curves with ∇ , $*$, Δ , and \diamond correspond to 6, 4, 3, and 2 periods of the B lattice, respectively. Curves for barriers with more than six lattice periods practically coincide with the curve for six periods). Note that for the relatively large barrier width the effective mass m_B^* monotonically increases with energy, being close to $m_1 = 0.022m_0$ for energies close to the conduction-band minimum of the

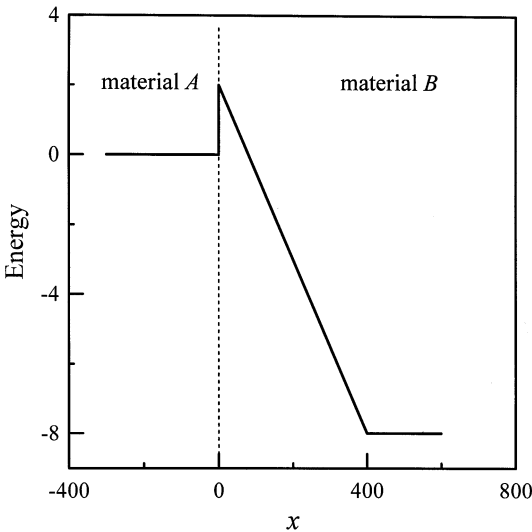


Fig. 2. Schematic of the potential energy profile used to simulate the triangular potential barrier. The two lateral unaffected materials are considered to be infinite.

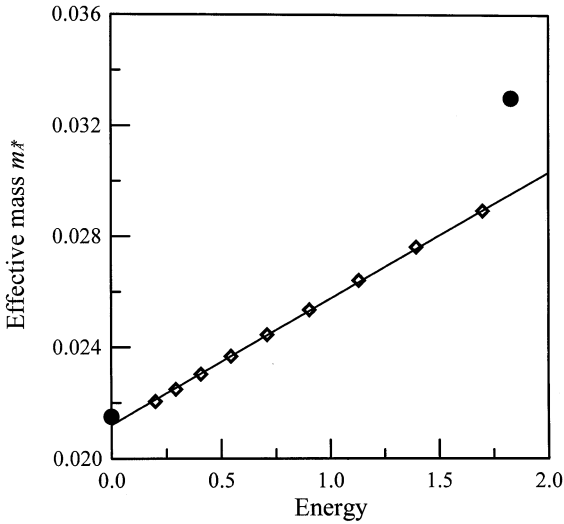


Fig. 3. Behavior of m_A^* of the well material of the well (diamonds) as a function of energy. A linear fit (solid lines) which reproduces very well the dependence of m_A^* on energy for the whole energy range is also shown.

A lattice, tending to reach m_2 as the energy approaches the conduction-band minimum of the B lattice. At an energy well below the barrier conduction-band edge, the effective mass m_B^* of the tunneling electrons is considerably lower than the bulk-conduction-band value of $m_2 = 0.033m_0$. The same conclusion was reached by Brozak et al. [4], analyzing the experimental results of tunneling cyclotron resonance in a thin barrier GaAs/AlAs superlattice. It was shown that the mass in the AlAs barrier is strongly renormalized down to $0.09m_0$ from the bulk-conduction-band value of $0.015m_0$ [4]. It seems that this kind of renormalization of the effective mass deep in the band gap is a general result and is connected with the density of states in the barrier region. We numerically verified that the behavior of the average density of states versus energy is qualitatively the same as for the effective mass, and therefore do not plot the corresponding figure to avoid repetition. For a very thin barrier, when the decay length of tunneling electrons becomes of the same order as the barrier width (see the curve with \diamond in Fig. 4), an anomalous increase of the effective mass is observed for high

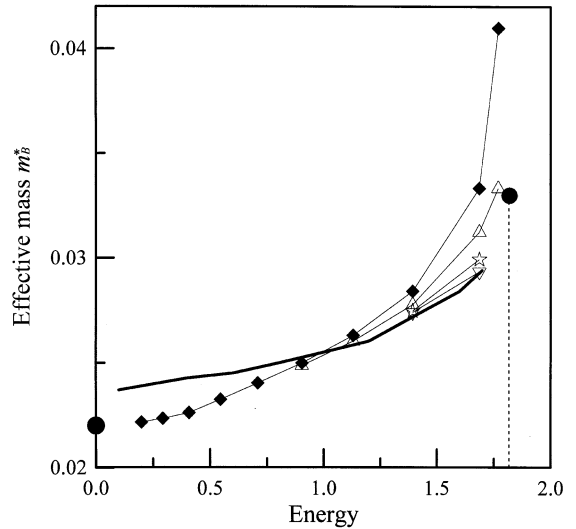


Fig. 4. Behavior of m_B^* of the barrier material as a function of energy for different barrier widths. The energy range is the height of the barrier, and the different barrier widths are, in periods of lattice B, 6 (V), 4 (*), 3 (Δ) and 2 (\diamond). In addition, we show as a solid line the behavior of m_B^* in the same range of energy, but for a triangular potential barrier.

energies. This can be interpreted as resulting from the formation of a very narrow band (and thus a very large effective mass) in the real part of the band structure in the barrier. It is also interesting to note that the behavior of the two masses, m_A^* and m_B^* , is quite similar, as can be seen by comparing Figs. 3 and 4. Hence, dividing by the effective mass in the boundary condition (2) does not significantly affect the results.

4.2. Triangular barrier

The solid line in Fig. 4 reflects the behavior of the effective mass of a tunneling electron in B, in which there is an applied electric field. It can be seen that m_B^* increases monotonically with energy, but with a lesser slope. This behavior is reasonable since in the triangular barrier there is always a region where the energy is very close to the conduction-band edge of material B.

It is of interest to emphasize here the great influence of material A on m_B^* , since this is

rarely taken into account. An example of current high-technological interest is the triangular or trapezoidal barrier which appears in a Metal–Oxide–Semiconductor structure, where both Fowler–Nordheim and direct tunneling are observed. The effective mass in the oxide is often measured by analyzing tunneling results [19,20]. In most of these studies the effective mass of the electron in the SiO₂ while tunneling is attributed only to the oxide material. According to the results of this paper, the effective mass in the emitter material, normally silicon, must also be taken into consideration as it can be dominant due to the substantial barrier height of the silicon–SiO₂ interface.

5. Conclusions

One of our foremost conclusions is that in computing transmission through a potential barrier, using constant values such as m_1 and m_2 is not a suitable approximation. An energy- and barrier-width dependent effective mass must be considered. If this is not done, the energy resonant peaks in a double-barrier system cannot be accurately obtained. Furthermore, the effective mass within the barrier, corresponding to energies within the bandgap in the barrier material, seems to be strongly influenced by the emitter material. This effective mass is closer to the conduction-band effective mass of the emitter material than to the effective mass in the conduction band of the barrier material at low energies, where tunneling takes place in many cases of interest. Another conclusion is that using a suitable energy-dependent effective mass that is independent of the barrier width can produce reasonably good results only down to about four lattice periods, and for energies that are not near the top of the barrier. For thinner barriers a strong deviation is observed, mainly at high energies, while almost no deviation is seen at very low energies. The coincidence of the effective mass values at very low energies, even with very narrow

barriers, is proof of the minimal influence of the barrier material in this energy region.

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