Transmission of electrons with flat passbands in finite superlattices

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Abstract. Using the transfer matrix method and the Ben Daniel-Duke equation for variable mass electrons propagation, we calculate the transmittance for symmetric finite superlattices where the width and the height of the potential barriers follow a linear dependence. The width and height of the barriers decreases from the center to the ends of the superlattice. The transmittance presents intervals of stopbands and quite flat passbands.

1. Introduction
The subject of propagation of any kind of waves in layered structures is very important. One of their important applications is as reflector structures and as filters. The search for energy, electronic, optical and acoustic filters is an interesting and active field. Formerly the transmittance for a superlattice where the barriers height is modulated by a Gaussian was calculated and very flat passbands are obtained [1]. In this work we propose a symmetric structure where the width and the height of the potential barriers follow a linear profile. The highest and widest barrier is at the center of the superlattice and the lowest or narrowest ones are at the ends. The idea behind using these types of structures is that it provides a slowly varying potential for the layers, which can improve the transmission of electrons through the multilayer system. For the calculations we use the transfer matrix method and the Ben Daniel-Duke equation for variable mass electrons [2]. The spectrum of transmittance of the structure presents stopbands and nearly flat transmission bands of energy. We compare this transmittance with that produced by a regular superlattice where all the barriers have the same height and width, and also for an inverted structure where the barriers width increases from the center to the ends.

2. Method
The propagation of the electrons in the structure is described by the Ben Daniel-Duke equation, appropriate for electrons with variable effective mass \( m^* \).

\[
\frac{-\hbar^2}{2} \frac{d}{dz} \left\{ \left( \frac{1}{m^*(z)} \right) \frac{d\psi(z)}{dz} \right\} + V(z)\psi(z) = E\psi(z)
\]  

(1)

The boundary conditions are the continuity of \( \psi(z) \) and \( 1/m^*(d\psi/dz) \). In order to solve the previous equation for our structures, we use the formalism for transfer matrix and transmission coefficient of Pérez-Alvarez and Rodriguez-Coppola [3].

We consider a superlattice made with the materials \( GaAs / Al_xGa_{1-x}As \). We take the \( GaAs \) gap as 1.42 eV. We consider an \( AlAs \) concentration until \( x=0.45 \) for which \( AlGaAs \) has still a direct gap of 1.98 eV. The conduction band offset for the \( GaAs / AlGaAs \) interface is 0.6. The maximum height which can be taken for the barriers is 0.33 eV corresponding to a concentration \( x=0.45 \). The width of
barriers and wells is given in monolayers, one monolayer (ML) has a thickness of 2.825 Å. In order to calculate the electron effective mass \( m \) for the alloy, we use the virtual crystal approximation [4], with

\[
\frac{1}{m_i} = \frac{x_j}{m_A} + \frac{1 - x_j}{m_G}
\]

\( m_A \) and \( m_G \) being the electron effective masses for pure AlAs and GaAs, which we take respectively as 0.15 and 0.067 of the free electron mass. With this approximation the concentration is given by \( x = V / 0.733 \), where \( V \) is the height of the barriers for the superlattice.

3. Results
We consider superlattices where the height or the width of the barriers follows a symmetric linear variation where the highest or widest barrier is at the center, and the lowest or narrowest ones are at the ends of the structure. The well width is constant for a particular structure. Fig. 1 presents the transmittance versus energy of the incident electrons for two types of structures with 13 barriers. \( V_{\text{max}}, V_{\text{min}} \) are respectively the maximum and minimum height of barriers, while \( h_{\text{max}}, h_{\text{min}} \) are the maximum and minimum width of barriers considered. One structure has only variation of the barriers height and the other one has both variations of height and width.

![Figure 1. Transmittance vs. energy, 13 barriers. Dashed curve: only height barriers modulation, \( V_{\text{max}}=0.33 \text{ eV}, V_{\text{min}}=0.047 \text{ eV}. \) Solid curve: also with width barriers modulation, \( h_{\text{max}}=5 \text{ ML}, h_{\text{min}}=2 \text{ ML. Well width}=22 \text{ ML.} \)](image)

Fig. 2 shows also the transmittance for two types of structures with 13 barriers with another set of parameters for the barriers and wells. One structure has only variation of the barriers width and the other one has both variations of width and height. The flat passbands are outstanding for Figs. 1 and 2.
Figure 2. Transmittance vs. energy, 13 barriers. Dashed curve: only width barriers modulation, \( h_{\text{max}} = 7 \text{ ML}, h_{\text{min}} = 1 \text{ ML}, V = 0.15 \text{ eV} \). Solid curve: also with height barriers modulation, \( V_{\text{max}} = 0.15 \text{ eV}, V_{\text{min}} = 0.09 \text{ eV} \). Well width=20 ML.

Fig. 3 shows in solid line the transmission for a superlattice with barriers of height of 0.20 eV and variable width; the wells width is 20 ML. For comparison we present in dashed line the transmission of a regular superlattice where the 13 barriers have the same width of 7 ML.

Figure 3. Transmittance vs. energy, 13 barriers, \( V = 0.20 \text{ eV} \), wells width=20 ML. For the solid curve the barriers width is \( h_{\text{max}} = 7 \text{ ML}, h_{\text{min}} = 1 \text{ ML} \). The dashed curve is the transmittance for a regular structure with the same width of 7 ML for all the barriers.

We stress the flatness of the passband for the superlattice with a linear variation of the barriers width in opposition to the transmission for the regular structure. The passband for the regular superlattice has oscillations which are the curves of resonance for the eigenenergies due to the 12 wells.
Figure 4. Transmittance vs. energy, 13 barriers, $V=0.20$ eV, wells width=20 ML. Solid curve is transmittance for the inverted linear superlattice with $h_{\text{min}}=1$ ML at the center of the structure and $h_{\text{max}}=7$ ML at the ends. Dashed curve is transmittance for the regular superlattice of Fig. 3.

The decrease of the barrier width from the center toward the sides of the structure causes a drop of the lifetime $\Delta t$ for the eigenstates, due to the fact that the electrons tunnel more easily. For the uncertainty principle $\Delta E \Delta t \geq \hbar/2$, the resonance bandwidth $\Delta E$ increases and the passband, which is the envelope of the resonance curves, becomes flatter. Finally, Fig. 4 presents the transmittance for the regular structure of Fig. 3 and the transmittance for an inverted superlattice with an opposite linear variation of the barriers width, where the narrowest barrier is at the center of the structure while the widest ones are at the ends. For this last structure the electrons are more confined that in the regular structure and the resonance peaks are narrower.

4. Conclusions
We have made a study of the electrons transmittance for a finite superlattice where the height and width of the potential barriers follows a linear profile. The highest or the widest barrier is at the center of the structure and the lowest or thinnest ones are at the ends. The transmittance presents flat transmission and reflection bands. This type of structure could have applications as energy filters for electrons, allowing electrons of a selected energy interval to pass through. This superlattice could also be suitable for superlattice solar cells. For this purpose we plan to do calculations for these structures subject to an electric field.

References
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