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Physica E 7 (2000) 832–835

PHYSICA E

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Gaussian semiconductor superlattices

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Abstract

We study GaAs-Al_xGa_{1-x}As superlattices where the heights of the barriers are modulated by a Gaussian profile. Such structures present bands of almost unscattered electronic states. The calculated energy levels of the superlattice agree well with the photoluminescence spectra recorded at low temperature. © 2000 Elsevier Science B.V. All rights reserved.

PACS: 68.65.+g; 73.20.Dx; 73.61.−r

Keywords: Superlattices; Electron transmission; Photoluminescence; Disorder

1. Introduction

Discussion of electron transport in semiconductor superlattices (SLs) can be traced back more than quarter a century to the pioneering work by Esaki and Tsu [1]. Owing to progress in crystal availability and epitaxial growth technology, it is possible to tailor the band structure of SLs to the particular needs of every experiment [2]. This makes SLs ideal candidates to carry out basic experiments to allow for a clear-cut validation of theoretical results, like Anderson localization in low-dimensional systems [3] and delocalization by correlated disorder [4]. In this context, Tung and Lee [5] proposed a novel SL where the heights of the barriers *and* the bottom of the quantum wells are modulated by Gaussian functions. These authors found some plateaus in the transmission coefficient where electrons are almost unscattered. This is quite different from the transmission characteristic in *uniform* SLs with Kronig–Penney profile, where the transmission probability is not uniformly equal to unity within each miniband. Recently, we have reported similar effects in GaAs-Al_xGa_{1-x}As SLs where only the barriers are modulated, whereas the wells are made of the same semiconductor and found that the j–V characteristic presents negative differential resistance with peak-to-valley ratios much greater than uniform SLs [6]. This design requires smaller values of the Al mole fraction in the barriers, leading to smaller number of growth defects (recall that disorder leads

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PII: S1386-9477(00)00071-0

to localization of electrons and hence reduces the transmission probability [7]).

To validate the above-mentioned purely theoretical considerations we have grown by means of molecular beam epitaxy a new class of semiconductor superlattices, the so-called Gaussian SL. The sample has been characterized by photoluminescence (PL) techniques at low temperature. As a major point, we have found that the calculated energy levels agree well with the PL spectra, thus supporting our previous claims [6].

2. Theoretical considerations

Before discussing the experimental results, we present a brief overview of the theoretical results we have obtained to highlight the differences of Gaussian SLs as compared to *uniform* SLs. We consider a GaAs-$Al_xGa_{1-x}As$ SL and focus on electron states close to the band edges and use the effective-mass approximation. The electron and heavy-hole effective-masses throughout the structure are given by $m_e^* = m(0.067 + 0.083x)$ and $m_h^* = m(0.62 + 0.14x)$, respectively, m being the free electron mass [8]. To describe a Gaussian SL we modulate the Al fraction according to $x_0 \exp(-z_b^2/\sigma^2)$, where z_b denotes the coordinate of the center of every $Al_xGa_{1-x}As$ layer along the growth direction. The origin of coordinates is set at the center of the innermost barrier. Therefore, x_0 is the Al fraction at the central $Al_xGa_{1-x}As$ layer. In our calculations we have taken σ to be 28.875 nm and $x_0 = 0.468$. Therefore the height of this barrier is $V_0 = 0.35$ meV. The width of the barriers is $d_b = 1.5$ nm and the width of the wells is $d_w = 6.2$ nm. The corresponding effective-mass equation can be easily solved using standard transfer-matrix techniques [6].

It is quite important to elucidate whether or not moderate degrees of unintentional disorder destroys the expected plateaus where the transmission coefficient is close to unity. Thus, to improve our previous model, we now take into account unintentional imperfections occurring during growth. We simulate local excess or defect of monolayers by allowing the widths of the quantum wells to fluctuate around their nominal values d_w. Therefore, the width of the nth quantum wells is taken $d_w(1 + W\varepsilon_n)$, where ε's are random numbers uniformly distributed in the interval $[-\frac{1}{2}, \frac{1}{2}]$. Here W is a positive parameter measuring the fluctuations of the widths. In doing so, each quantum well presents a slightly different value of its thickness and, as a consequence, resonant coupling between electronic states of neighboring wells decreases [9]. The recourse of the transfer-matrix method allows us to obtain the transmission coefficient even if disorder is present in the model. Fig. 1 shows the transmission coefficient for the Gaussian SL with 15 barriers for $W = 0$ (perfect SL) and $W = 0.07$ (imperfect SL with fluctuations of the order of one monolayer). As expected, the transmission coefficient decreases upon introducing disorder but the main features are *robust*, namely the plateaus are still flat and the value of the transmission coefficient is quite close to unity. It is worth noticing that transmission coefficient is not uniformly equal to unity within each miniband in *uniform* SLs, even if disorder is neglected (see, e.g., Ref. [6]). Therefore, we are led to the conclusion that moderately disordered Gaussian SLs present better transmission properties than perfect uniform SLs.

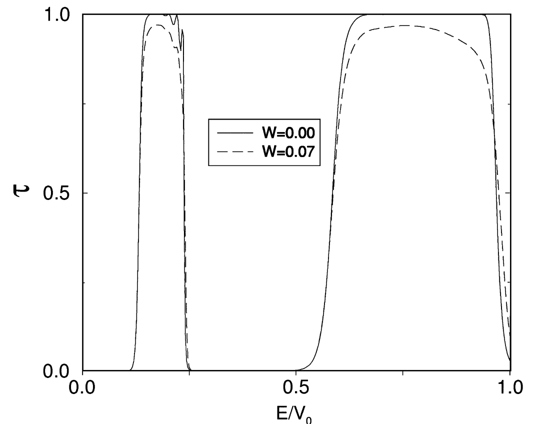

Fig. 1. Transmission coefficient as a function of the reduced energy E/V_0 for the Gaussian SL without disorder (solid line) and including disorder (dashed line). Notice the occurrence of two bands below the highest barrier.

3. Experimental results

Having discussed the features expected in Gaussian SL we now proceed to discuss the experimental results. The Gaussian SL with the parameters given in the previous section has been grown by molecular

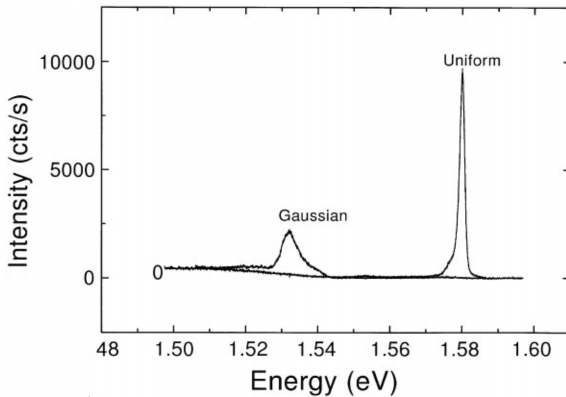

Fig. 2. PL spectra of Gaussian and uniform SLs recorded at 4 K.

beam epitaxy. In order to highlight the peculiarities of the Gaussian SL, we have also grown a uniform SL with 15 barriers of the same width and Al fraction x_0 and compared the results. In each sample, the SL is cladded on each side by 100 nm of n-$Al_{0.3}Ga_{0.7}As$, Si doped to 4×10^{18} cm^{-3}, with a 50 nm n-GaAs buffer layer (doped to 4×10^{18} cm^{-3}) on the substrate and a 3 nm n-GaAs cap layer (doped to 6×10^{18} cm^{-3}).

PL spectra are shown in Fig. 2 for both SLs. The peak of the PL intensity from the uniform SL is about 1.58 eV while that corresponding to the Gaussian SL is located close to 1.53 eV. This shift is clearly due to the different electronic structure of both SLs. To further support this claim we have performed self-consistent calculations of the electronic structure of both SLs using the effective mass Schrödinger equation within the envelope function framework and the Poisson equation [10]. For brevity we only present the results for the Gaussian SL in Fig. 3,where the ground and first excited states for both electrons and heavy holes are shown. The energy difference of the conduction- and valence-band states are rather close to 1.53 eV, in agreement with the PL results presented in Fig. 2. The same calculations in the uniform SL yield the energy difference close to 1.58 eV, again in perfect agreement with the PL results.

To conclude, we have presented a new design of a band-pass filters using Gaussian SLs. The obtained transmission probability is almost equal to unity within the allowed minibands. To ascertain the validity of our theoretical predictions, we have grown Gaussian and uniform SLs by molecular beam epitaxy

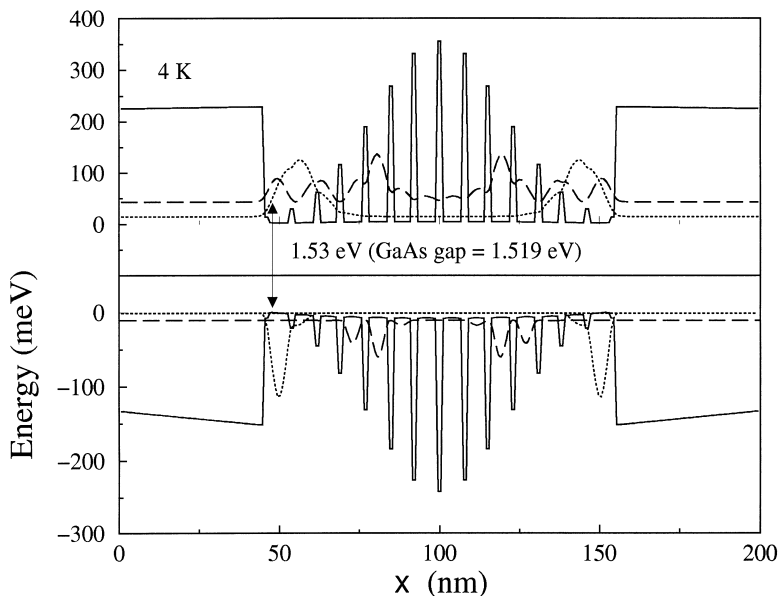

Fig. 3. Electron and hole levels of the Gaussian SL at 4 K. Dotted (dashed) lines indicate the ground (excited) states of electrons and heavy holes. The self-consistent potential is indicated by the solid line.

methods. The PL spectra recorded at low temperature are in agreement with the electronic structure calculated self-consistently. According to our predictions, Gaussian SLs should present much higher values of the peak-to-valley ratio in the *j–V* characteristics. Our preliminary transport measurements suggest that this is certainly the case. Work along this direction is currently in progress.

Acknowledgements

Work at Madrid and Pavia has been supported by CAM (Spain) under Project No. 07N/0034/1998, DGES AA.II. Spain-Italy and the INFM Network "Fisica e Tecnologia dei Semiconduttori III-V". E.D. was supported by the Spanish Ministry of Education and Culture.

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