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Interface roughness effects in Gaussian superlattices

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Abstract
We investigate the effect of unintentional disorder on the pass-band capabilities of a GaAs–$Al_xGa_{1-x}As$ superlattice with Gaussian modulated Al mole fraction. We prove that if fluctuations of vertical disorder can be kept below two monolayers the pass-band filter capabilities are not severely degraded. In addition Al fluctuation as encountered in typical molecular beam epitaxy growth conditions does not degrade the filter capabilities of the Gaussian superlattice. We introduce a new model to deal with lateral disorder and prove that in a molecular beam epitaxial growth process lateral disorder effects are negligible as compared with the vertical disorder ones.

The idea of creating solids that give rise to arbitrary potential profiles can be traced back to the 1970s. The pioneering conjecture of Tsu and Esaki [1] would have been useless though without a parallel progress in semiconductor heterostructure growth technology that, with the advent of molecular beam epitaxy (MBE), has made possible the birth of low-dimensional physics and a new generation of opto-electronics and electronics devices based on the concept of 'bandgap engineering'.

Among the devices that can be obtained with a semiconductor superlattice (SL), a desirable one would be a high-performance energy band-pass filter capable of transmitting only electrons lying in a given band. Such a device could serve in a number of applications. To mention just one let us consider the potentiality of an electronic band-pass filter in increasing the efficiency of a quantum cascade laser [2, 3]. In a quantum cascade laser the lasing action is due to electrons undergoing transitions between conduction subbands of an appropriate heterostructure. In a quantum cascade laser an electron confined in the active region emits a photon transiting from the confined higher state E_2 to the lower state E_1; the electron then exits the active region, tunnelling into the next active region, where the radiative process occurs again. The injection/relaxation SL on both sides of an active region should serve as an energy pass-band filter for electrons with energy E_1 and as a stop-band for electrons with energy E_2. The usually adopted injection/relaxation regions serve as filters with a pass-band and stop-band characterized by a transmission coefficient τ of the order of 10^{-1} and 10^{-4} respectively [4–6]. Clearly the efficiency of the lasing action could be much higher if the transmission coefficient for the pass- and stop-band could be unity and zero respectively.

A band-pass filter based on a GaAs–$Al_xGa_{1-x}As$ SL was first proposed by Tung and Lee [7], but was never fabricated because the current state of the art of MBE does not permit us to grow it with an acceptable number of defects. Recently Gómez *et al* [8] proposed a new electron band-pass filter design, also based on GaAs–$Al_xGa_{1-x}As$, the so-called Gaussian SL (GSL), that allows for better crystallographic qualities than the one proposed in [7]. This proposal allows the device to be built with a limited number of defects due to the smaller mole fractions involved in the design of the heterostructure [8]. The GSL is a quantum well based SL, where only the barrier heights are modulated, by a proper choice of the Al fraction x, according to the modulation function $V_o \exp[-(z_b^n)^2/\sigma^2]$, where z_b^n is the coordinate along the growth direction of the nth barrier midpoint and V_0 is the maximum height of the potential barrier entering the heterostructure. The proposal appears very interesting but the model used to investigate electron transport through the structure describes a far too ideal situation. A certain amount of unintentional disorder is always introduced in the heterostructure growth process and this fact is well known to have deep effects on the transport properties of semiconductor heterostructures [4–6]. In the case of the GSL, a small amount of unintentional disorder could be particularly critical as far as the pass-band peculiarity is concerned, this also in view of the thinness of the barriers that constitute the GSL. In fact, the barriers' width as proposed by Gómez *et al* [8] is 1.5 nm. It is then important to estimate to what extent the striking properties of the GSL are robust and what should

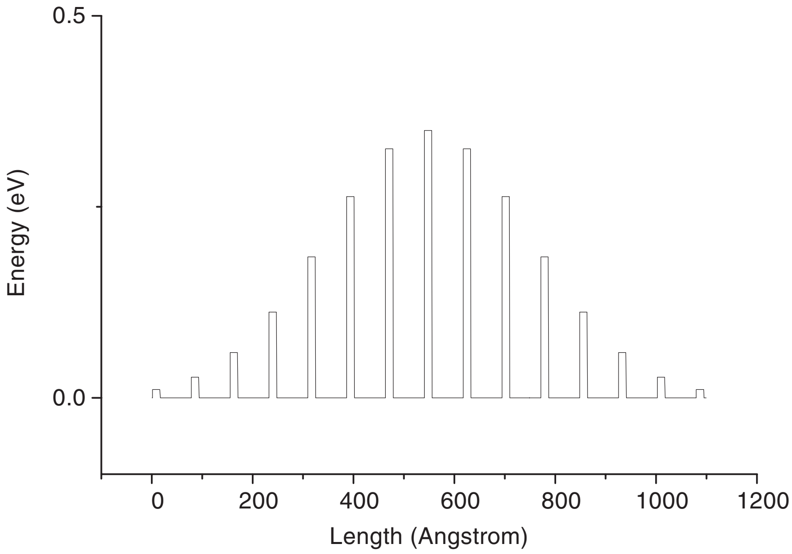

Figure 1. Profile of the conduction band energy of the Gaussian SL. The parameters used are as in the calculation.

be the accuracy of the fabrication parameters. Modern MBE equipment allow the growth of modulated SLs; recently we grew and studied experimentally [9] a GSL with the structural and geometrical parameters proposed by Gómez *et al.*

Disorder is not the only scattering mechanism. In principle, in the ballistic regime, the potential profile felt by an impinging electron can be modified as well by the electron–electron interaction. The effect of the electron–electron interaction on the transmission coefficient of the GSL has been explored in [9, 10], performing a self-consistent calculation of the Schrödinger and Poisson equations, and was found not to affect the band-pass characteristic of the device.

In this paper we report on the effect of unintentional disorder on the transmission properties of the GSL. We adopted a statistical approach in treating disorder in SLs as related to the transport properties. We introduce a simple model, which should hold in many cases, to account for lateral disorder. We find that, for the typical parameters of a GSL, fluctuations of two monolayers in the barrier thickness do not appreciably modify the transmission curve.

Unintentional disorder in SLs can be classified into two categories: lateral and vertical [11]. Vertical disorder occurs whenever the layer thickness or the mole fraction of the chemical species forming the alloy (Al fluctuation in $Al_xGa_{1-x}As$ in the case of the GSL) fluctuate around their nominal values. Vertical disorder destroys the periodicity of the SL along the growth direction. We have lateral disorder whenever semiconductor A protrudes into semiconductor B (and vice versa), forming chemically intermixed interfaces, steps and islands. This kind of disorder yields a rough interface where transitional symmetry in the plane perpendicular to the growth direction is broken. Both kinds of disorder take place in the growth process.

We start by considering vertical disorder. We model the deviation of the layer thickness by allowing w_b^n and w_w^n (the width of the nth potential barrier and of the nth quantum well, respectively) to fluctuate around their nominal values, w_b and w_w, according to

$$w_b^n = w_b(1 + W\varepsilon_n) \tag{1}$$

under the constraint $w_b^n + w_w^n = w_b + w_w$. W is a positive parameter which measures the maximum fluctuation while the ε_n are uncorrelated random numbers of magnitude smaller than $1/2$. More precisely, denoting by $P(\varepsilon_n)$ the probability of the occurrence of ε_n, we assume

$$P(\varepsilon_n) = \begin{cases} 1, & \text{if} \quad |\varepsilon_n| < \frac{1}{2} \\ 0, & \text{otherwise.} \end{cases} \tag{2}$$

The same procedure will be adopted to describe Al mole fraction fluctuations: $x^n = x_0^n(1 + Y\varepsilon_n)$, hence $V_b^n = V_0^n(1 + Y\varepsilon_n)$, where x^n is the Al mole fraction value of the nth layer of $Al_xGa_{1-x}As$ and x_0^n is its nominal value, V_b^n is the height of the nth potential barrier while V_0^n is its nominal value and Y is a positive parameter that controls the maximum allowed fluctuation [12]. For simplicity we disregard, for the moment, Al mole fraction fluctuations.

A given W and a given sequence $\{\varepsilon_n\}$ identify uniquely a SL and hence a potential profile. Formally, as far as the transport properties in the ballistic regime are concerned, the SL is described by a transmission coefficient $\tau(E)$ where $E = \hbar^2 k_z^2/2m^*$ is the energy component of the electron along z, the growth direction, and m^* the effective mass in the conduction band. We calculate the transmission coefficient by making use of transfer matrix techniques as in [13]. We shall give a statistical description of the transmission properties. To this end we proceed as follows: (a) we 'build' M random potential profiles by choosing M sequences $\{\varepsilon_n\}$ and we calculate the corresponding transmission curves $\tau_i(E)$, with $i = 1, \ldots, M$; (b) we calculate, for each value of the energy E, the mean value $\bar{\tau}$ and the standard deviation $s(E)$ of the transmission.

The data reported here were calculated for a GSL with the following parameters (see figure 1): maximum barrier height $V_0 = 0.35$ eV; $\sigma = 28.875$ nm; number of $Al_{0.3}Ga_{0.7}As$ barriers $= 15$; barrier width $w_b = 1.5$ nm and well width $w_w = 6.2$ nm for a total length of 109.3 nm. The total length is sufficiently small to ensure that the electron transport takes place in the ballistic regime as recently shown in [14]. With these parameters and no applied voltage, the ideal GSL

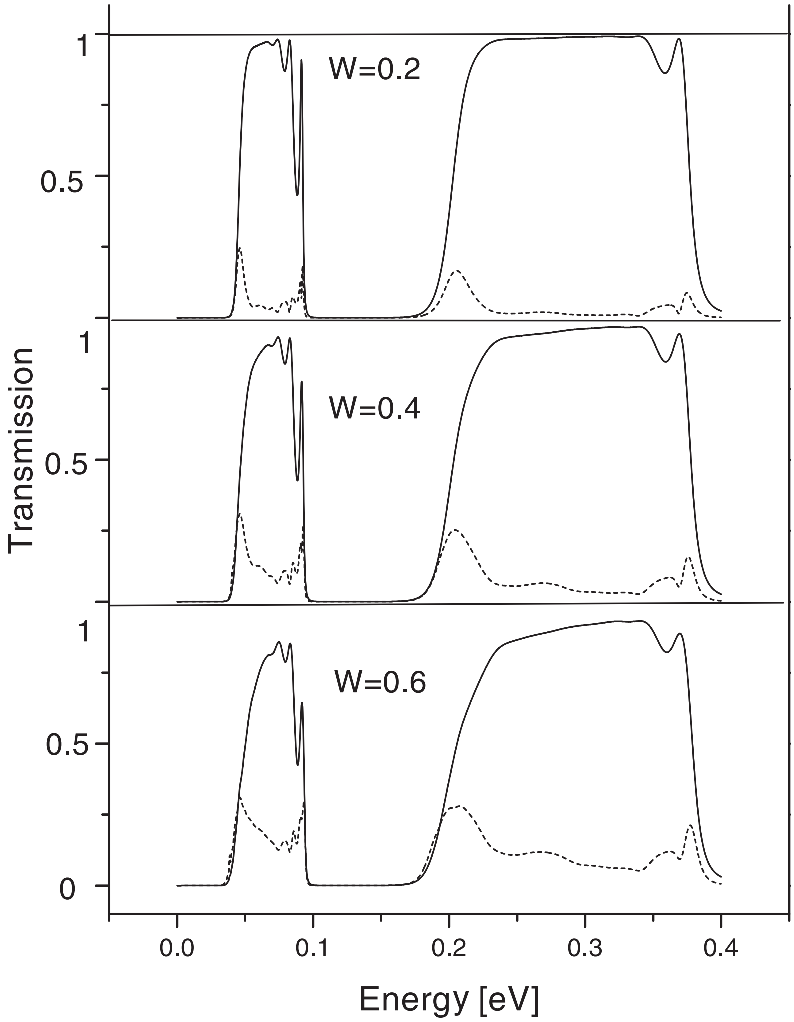

Figure 2. Effect of vertical disorder in Gaussian SLs. Solid curve, average transmission. Dashed curve, standard deviation. Calculations are performed with the disorder parameter W as specified in the figure.

transmits electrons with energy in the two bands, one between 0.04 and 0.1 eV and another one between 0.25 and 0.37 eV. We performed the calculations with various amplitudes of the maximum fluctuation W. For each W we used $M = 100$. In figure 2 we report the average transmission $\bar{\tau}(E)$ and the standard deviation $s(E)$ for $W = 0.2$, 0.4 and 0.6. We notice that $M = 100$ is sufficiently large to give a statistically reliable description. Indeed we calculate that one has 99.7% probability that the true average $\langle\tau\rangle$ is within the following range: $\left[\bar{\tau} - 3\frac{s}{\sqrt{M}}; \bar{\tau} + 3\frac{s}{\sqrt{M}}\right]$. With $M = 100$ such an interval is of insignificant width as compared to the standard deviation. Figure 2 clearly shows that the striking features of a sharp pass-band filter remain up to $W = 0.4$. As W increases further, the features start to be lost. At $W = 0.4$, for the case here considered, the corresponding maximum fluctuation of the barrier thickness is 6 Å. This is about the thickness of two monolayers, which are deposited during the fabrication process. The curve of the standard deviation shows that the variation of the transmission from sample to sample has its peaks at the edges of the bands. In the middle the transmission is less affected. What the standard deviation does not show is whether, for a given sample with vertical disorder, the transmission at the onset of the pass-bass is smooth or oscillates. The transmission in a few selected cases is shown in figures 3(a) and (b). These graphs clearly elucidate the destructive effect of disorder. We also notice how the effect of disorder does not imply the occurrence of oscillations in the transmission coefficient pass-band region or at the onset of the pass band. We stated earlier that $W > 0.4$ greatly reduces the filter capabilities of the GSL. This is true if we compare the graph of figure 3 relative to $W = 0.6$ versus the one corresponding to $W = 0.4$. Actually the performance for a disorder parameter $W = 0.6$ is still much better than what can be expected from other potential profiles even in the absence of disorder, such as that of a uniform SL of 15 barriers and 14 wells [8] or the potential profile used as injection/relaxation region in quantum cascade lasers [4, 6].

As already mentioned, disorder can be lateral as well. We neglect for the time being any vertical disorder, which means that for any sample the thickness of each layer can change in the transverse plane but its average coincides with the nominal one. It is quite difficult to make a prediction in a general case of lateral disorder since the problem is fully three dimensional. However we can simplify the problem when D, the transversal average dimension of protrusions, is not particularly small. To this end we divide the SL into Q channels of transversal

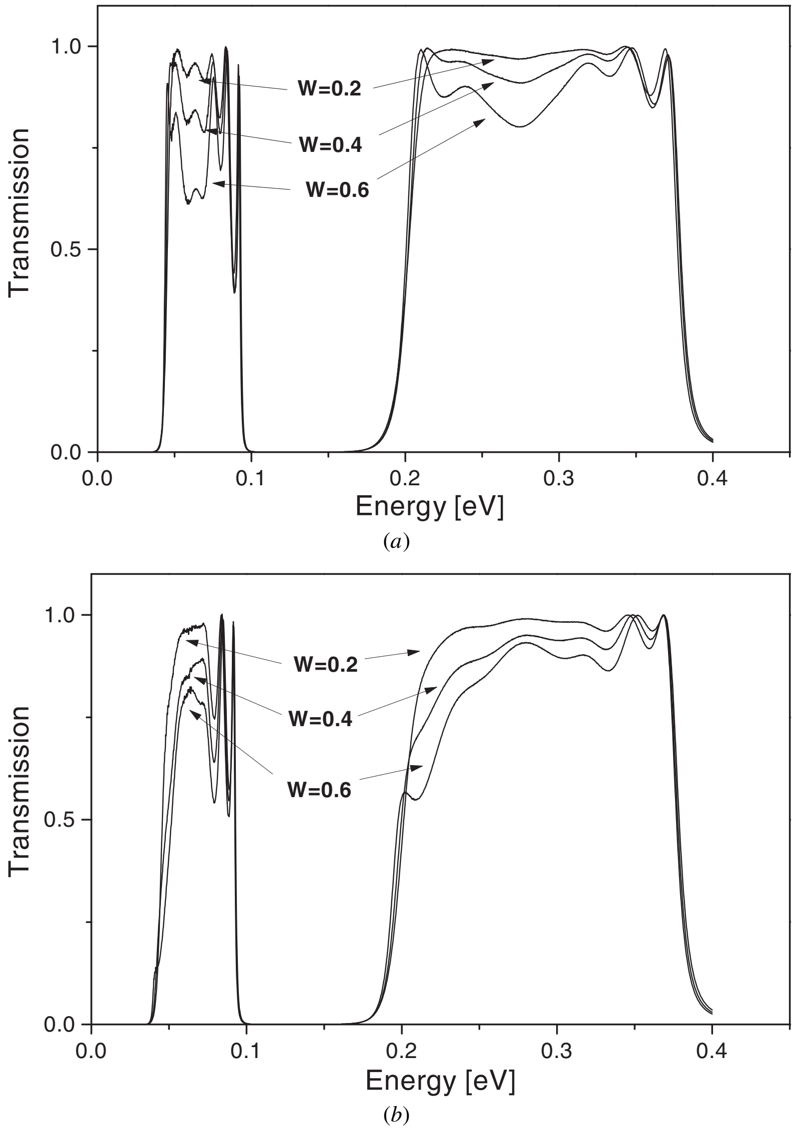

Figure 3. Transmission coefficient in two specific cases, (*a*) and (*b*), of vertical disorder. In each of the two figures we kept the same sequence $\{\varepsilon_n\}$ and varied the disorder parameter W.

dimension d. If we choose d such that $d < D$ each channel appears to the impinging electron as transversally uniform. The situation is shown in figure 4. We then ignore diffraction of the impinging electron wave out of a channel. This requires

$$\frac{\lambda_e}{d}L < d \tag{3}$$

where L is the length of the SL and λ_e the electron wavelength. Equation (3) originates from wave optics and it is a limitation for the size of the Fresnel zone. We notice that under this approximation no interference phenomena occur among different channels. With $L \sim 100$ nm and an electron energy $E_z \sim 0.04$ eV, equation (3) is fulfilled for $d \sim 50$ nm. Within each channel the transport problem is now cast in terms of vertical disorder: each channel has sharp barrier/well edges and its transmission coefficient τ_{CH} can be calculated as before from the thicknesses of barriers and wells. Assuming the SL to be divided into Q equal channels, the transmission coefficient of a specific laterally disordered SL is then

$$\tau_L = \frac{1}{Q}\sum_{i=1}^{Q}\tau_{CH,i} \tag{4}$$

where $\tau_{CH,i}$ is the transmission coefficient of the ith channel. Again, we characterize the distribution of the transmissions of the laterally disordered SLs through its average $\bar{\tau}_L$ and its standard deviation s_L. The latter quantities, by making use of the their definition and of equation (3), can be expressed through $\bar{\tau}_{CH}$ and s_{CH}, the average and standard deviation of the transmission of a single channel. We obtain $\bar{\tau}_L = \bar{\tau}_{CH}$ and $s_L = s_{CH}/\sqrt{Q'}$, where Q' is the number of uncorrelated channels. Since the transverse size of the area where the thickness remains correlated is about D, one has that $Q' \approx$ total area$/D^2$.

Vertical disorder has a deeper impact on the transmission characteristic as compared to lateral disorder. In fact, even though the average transmission curve is practically the same in

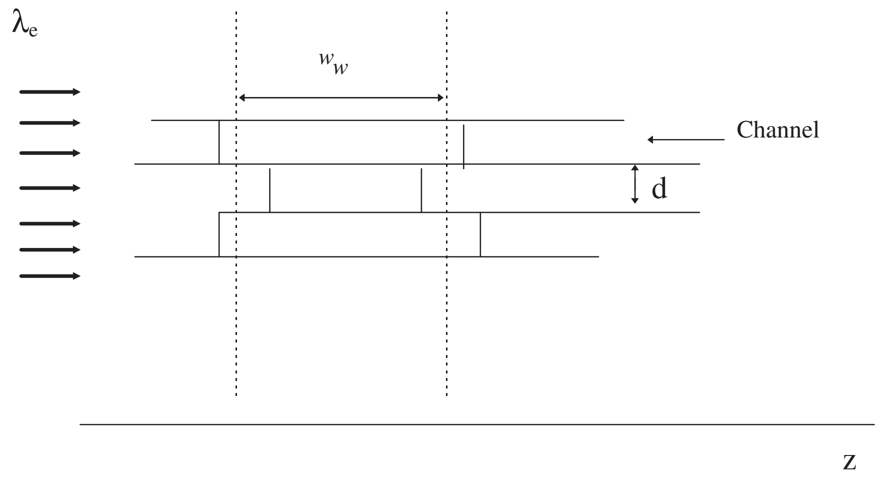

Figure 4. Partition of the SL into Q channels of transversal dimension d. If we choose d such that $d < D$, the transversal average dimension of protrusions, each channel appears to the impinging electron as transversally uniform. The arrows represent the impinging electron, λ_e is the impinging electron wavelength, $w_w$is the nominal barrier width and z is the SL growth direction.

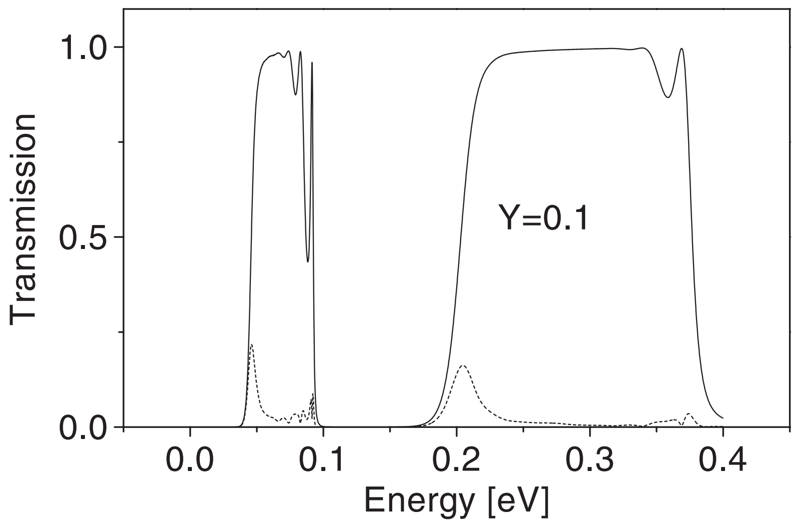

Figure 5. Effect of Al fluctuations in Gaussian SLs. Solid curve, average transmission. Dashed curve, standard deviation. Calculations performed with the disorder parameter Y as specified in the figure.

both cases of disorder, the standard deviation has greater values in the former case. To give an estimate, consider that typically an SL has lateral linear dimensions of the order of 100 μm [14]. Taking $D \sim 50$ nm we obtain a standard deviation for lateral disorder 10^4 times smaller than for the vertical disorder case.

The GSL transmission coefficient is robust, disorder becoming critical for $W > 0.4$ and, furthermore, in comparison with the reference SL results. Al mole fraction fluctuations do not infer the quality of the GSL. In fact, an Al fluctuation of 10%, a value much higher than that normally encountered in MBE growth process, does not change significantly the transmission coefficient as shown in figure 5.

Our results show that the band-pass filter characteristic of the GSL is not affected by unintentional disorder that may arise in the growth process as long as the barrier fluctuation can be kept below two monolayers. This makes us confident in a future use of such SL design in electronic devices. Furthermore we have established that, if interference among different channels can be ignored, vertical rather than lateral disorder has a leading role in affecting electron transport properties in SLs. This fact is important since it gives an indication to the crystal grower of what the main issue to work on to improve the MBE apparatus is. It also gives an indication to the theorist of when it becomes important to deal with lateral disorder using fully three-dimensional approaches, which are difficult both theoretically and numerically.

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