Interface-roughness-induced broadening of intersubband electroluminescence in *p*-SiGe and *n*-GaInAs/AlInAs quantum-cascade structures

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The effect of intrasubband interface roughness scattering on intersubband transition linewidths in double-quantum-well and quantum-cascade (QC) structures is studied. In *n*-GaInAs/AlInAs structures, the calculated ratios between the linewidths of the spatially vertical and diagonal transitions agree with the experimental values. In *p*-Si/Si_{0.2}Ge_{0.8} QC structures, the experimentally observed linewidth is a factor of 4–7 smaller than the predicted value. However, by assuming a vertical interface correlation between adjacent interfaces separated by less than ~ 1.5 nm, the theory reproduces the experiment. Transmission electron microscopy of the SiGe QC sample reveals this vertical correlation, supporting the model. © 2005 American Institute of Physics. [DOI: 10.1063/1.1862344]

SiGe quantum-cascade (QC) structures utilizing optical intersubband transitions are potentially important for efficient Si-based light sources.^{1–3} Strain-compensated SiGe structures, where the average Ge content of the epilayer is matched to that of a virtual substrate, allow the growth of a large number of active cells while increasing the band offset, providing sufficient design freedom.^{2,4} Recently, strain-compensated Si/Si_{0.2}Ge_{0.8} QCs with total thicknesses exceeding 1 μ m on Si_{0.5}Ge_{0.5} virtual substrates have shown electroluminescence (EL) centered at 175 meV². However, the observed linewidth is rather broad. In order to realize QC laser devices, optimization of the optical gain is crucial and linewidth broadening mechanisms have a detrimental effect. Previous study of low-temperature in-plane mobility in Si/Si_{0.2}Ge_{0.8} quantum wells (QWs) on Si_{0.5}Ge_{0.5} substrates has shown that the interface roughness scattering is the primary mobility-limiting process for wells below 4.5 nm.⁵ Therefore, we have studied the effect of interface roughness scattering on the broadening of the intersubband EL in strain-compensated QC structures and found it to be the dominant cause of the EL spectrum broadening. In comparison, optical phonon emission via the deformation potential interaction which limits the excited state lifetime to ~ 250 fs in midinfrared SiGe QCs,⁶ has a minor impact.

To model the effect of the interface roughness scattering, we calculate the dephasing rate of the intersubband transitions induced by the interface roughness scattering using the theory by Ando.^{7,8} The interface scattering potential for carriers in the *n*th subband due to the roughness $h_i(\mathbf{r})$ at the interface $z=z_i$, is written as $V(\mathbf{r}) = \delta U(z_i) |f_n(z_i)|^2 h_i(\mathbf{r})$, where $f_n(z)$ is the wave function, $\delta U(z_i) \equiv -\{U(z_i+) - U(z_i-)\}$ is the potential step, and $\mathbf{r}$ is the in-plane coordinate along the interface.^{9–12} We assume a standard Gaussian autocorrelation of the roughness $\langle h(\mathbf{r})h(\mathbf{r}') \rangle = \Delta^2 \exp(-|\mathbf{r} - \mathbf{r}'|^2/\Lambda^2)$ with an average roughness height Δ and a correlation length Λ along

the interface plane.¹³ The largest contribution comes from the intrasubband scattering. From the theory, this gives an intersubband broadening Γ for transitions between two parabolic subbands *n* and *m* in the limit of negligible carrier concentration as follows;

$$\Gamma = 2\pi^2 \rho \Delta^2 \Lambda^2 \sum_{ij} c_{ij} F_i F_j, \quad (1)$$

where F_i is equal to $\delta U(z_i) \{|f_n(z_i)|^2 - |f_m(z_i)|^2\}$, ρ is the density of states $m^*/(2\pi\hbar^2)$ with m^* denoting the in-plane effective mass, and c_{ij} represents the vertical correlation of the roughness between the *i*th and *j*th interface. Here, we assume that the interface roughnesses at different interfaces are characterized by the same Δ and Λ . c_{ij} is equal to 1 when $i=j$. When all of the interfaces are uncorrelated to each other, c_{ij} is zero for $i \neq j$. We note that when the vertical correlation is finite, Eq. (1) predicts partial cancellation of the roughness scattering, since F_i takes opposite sign between adjacent interfaces.

We first apply the theory to the well-established intersubband transitions in lattice-matched *n*-GaInAs/AlInAs structures on InP. In these structures, the vertical interface correlation between different interfaces can be neglected [c_{ij} is zero for $i \neq j$ in Eq. (1)] because of the high growth temperature and the lack of strain distribution.^{14,15} In the double-QW (DQW) depicted in Fig. 1(a) absorption can occur either via the diagonal transition between the first and the second state, or via the vertical transition between the first and the third state. Figures 1(d) and 1(e) show the measured low-temperature absorption of the diagonal and the vertical transitions, respectively. The 1-2 transition is observed at 97 meV with a Γ_{12} of 9.7 meV, and the 1-3 transition is observed at 335 meV with a Γ_{13} of 11.6 meV. Interface roughness has the strongest impact on the energy broadening of the third state because of the large amplitude of the wave function at the interface compared to the first two states. However, the large spatial overlap between the first and the third state partially cancels the effect and the theory predicts that

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FIG. 1. Band structure and wave functions of the lattice matched n -GaInAs/AlInAs structures on InP substrates: (a) The modulation-doped DQW with single-period layers of **3.0/3.0/3.5/1.0/4.7/3.5** from the left, where the GaInAs wells are in roman, the AlInAs barriers in bold and the doped layer ($\text{Si } 3 \times 10^{17} \text{ cm}^{-3}$) is underlined, (b) the diagonal transition QC structure (from Ref. 20), and (c) the vertical transition QC (from Ref. 21). Panels (d) and (e) show the absorption spectrum of the 60-period DQW sample measured at 15 K using a multipass waveguide geometry, corresponding to the diagonal 1-2 transition (d) and the vertical 1-3 transition (e), respectively. For the latter, a slowly varying baseline is subtracted for clarity.

the linewidths of the two transitions are approximately equal. This agrees well with the observed ratio Γ_{13}/Γ_{12} of 1.2. Note that the spectral shape of the absorption is also affected by nonparabolicity, electron-electron interactions,^{16,17} other scattering mechanisms, and disorder.^{18,19} The detailed consideration of these effects is beyond the scope of this letter.

Next, we consider the broadening of the EL spectra of the GaInAs/AlInAs QC structures having spatially diagonal and vertical transitions depicted in Figs. 1(b) and 1(c), respectively. Compared to the absorption in the DQW, in the case of EL from the QCs, the effect of the subband dispersion and the electron-electron interaction is weaker because of the smaller number of carriers ($\sim 10^{11} \text{ cm}^{-2}$ or less) involved in the process. The diagonal QC in Fig. 1(b) shows EL from the a to b intersubband transition centered at 185 meV at a bias of 70 kV/cm with a Γ_{dia} of 25 meV.²⁰ The EL peak of the vertical QC shown in Fig. 1(c) is centered at 160.2 meV with a Γ_{vert} of 7.5 meV.²¹ The improved linewidth of the vertical QC has been attributed to the smaller effect of the interface roughness than in the diagonal QC.²¹

FIG. 2. (a) Band structure and wave functions of the strain-compensated $\text{Si}_{0.2}\text{Ge}_{0.8}$ QC structure studied in Ref. 2 under forward bias with electric field of 70 kV/cm. (b) Transverse magnetic-polarized intersubband EL spectrum of a 15-period QC sample measured in the bias condition close to the emission threshold at 20 K.

From Eq. (1), the calculated linewidth ratio $\Gamma_{\text{vert}}/\Gamma_{\text{dia}}$ is equal to 0.23, in good agreement with the experimental value of 0.30.

By comparing calculation and experiment for the diagonal QC, we can evaluate the interface parameters of the GaInAs/AlInAs structures. The small contributions from the alloy²² and phonon scattering are neglected. The product $\Delta\Lambda$ is estimated to be 1.01 nm^2 . Using this value, we obtain the broadening of the other transitions as shown in the Table I. The overall agreement between the theory and the experiment is satisfactory. The corresponding interface parameters, for example $\Delta=0.17 \text{ nm}$ and $\Lambda=6 \text{ nm}$, are comparable to the reported values for GaAs and GaInAs,^{13,23} although a comprehensive study of the interface parameters is still needed for these materials.

Now we apply the theory to the SiGe QC structures.² Figure 2(a) shows the unit-cell band structure of the QC structure under a threshold bias field F of 70 kV/cm. The wave functions and the band structure are calculated using parameters evaluated by the method described in Refs. 24 and 25. Midinfrared radiation is generated by the intersubband transition of holes from a to b . Carriers are injected into a from the injector (c of the previous stage). Figure 2(b) shows the EL spectrum of a QC device consisting of 15 active cells. The linewidth Γ is equal to $41 \pm 5 \text{ meV}$ at a bias close to the emission threshold. The EL is measured at 15 K in a finger device geometry,² with $3 \mu\text{m}$ wide finger ridges to ensure current uniformity throughout the active layers. Further experimental detail and the current density dependence of the device will be described elsewhere.²⁶ The interface parameters $\Delta=0.4 \text{ nm}$ and $\Lambda=2.3 \text{ nm}$ of our SiGe structures have been determined previously.⁵ The in-plane effective mass $m^*=0.16 m_0$ calculated by six-band $\mathbf{k} \cdot \mathbf{p}$ theory (m_0 is the free electron mass) is used in this procedure. High-resolution cross-sectional trans-

TABLE I. Experimental (expt) and calculated (calc) linewidths of the electronic intersubband transitions in the GaInAs–AlInAs DQW and QC structures. For the linewidth broadening of the electroluminescent spectrum of the QCs are taken from footnotes a and b, respectively.

	Absorption (DQW)		EL (QC)	
Diagonal transition	$\Gamma_{12}(\text{expt})$ 9.7 meV	$\Gamma_{12}(\text{calc})$ 9.7 meV	$\Gamma_{\text{dia}}(\text{expt})$ 25 meV ^a	$\Gamma_{\text{dia}}(\text{calc})$ 25 meV
Vertical transition	$\Gamma_{13}(\text{expt})$ 11.6 meV	$\Gamma_{13}(\text{calc})$ 9.7 meV	$\Gamma_{\text{vert}}(\text{expt})$ 7.5 meV ^b	$\Gamma_{\text{vert}}(\text{calc})$ 5.63 meV

^aReference 20.

^bReference 21.

FIG. 3. (a) Calculated linewidth of the intersubband EL spectrum of the $\text{Si}_{0.2}\text{Ge}_{0.8}/\text{Si}$ QC structure limited by the interface roughness scattering. The linewidth was calculated as a function of the vertical correlation length κ . (b) Cross section of the sample imaged by the high-resolution TEM, showing the Si barriers (bright) and the $\text{Si}_{0.2}\text{Ge}_{0.8}$ wells (dark).

mission electron microscopy (TEM) [Fig. 3(b)] shows that these interface parameters are also consistent for the QCs. From the statistical analysis of the TEM cross section of this sample, we found for Δ a lower value of 0.32 ± 0.07 nm.

Using these interface parameters and Eq. (1), we find that the calculated Γ is equal to 170–300 meV, a factor of 4–7 larger than the experiment assuming that the different interfaces are uncorrelated. However, when we include the vertical correlation the calculated linewidth is significantly reduced. To evaluate the impact of the vertical correlation, we assume a Gaussian vertical correlation factor $c_{ij} = \exp[-(z_i - z_j)^2 / \kappa^2]$ with a vertical correlation length κ . Introducing this expression into Eq. (1), we calculate Γ as a function of κ and show the results in Fig. 3(a). For Δ equal to 0.3–0.4 nm and $\Lambda = 2.3$ nm, the linewidth observed in the experiment is reproduced for κ equal to 1.4–2.2 nm.

The vertical correlation of the interfaces can be observed in the TEM cross section of the sample [Fig. 3(b)]. Here, the bright regions represent the Si barriers separated by the $\text{Si}_{0.2}\text{Ge}_{0.8}$ wells. The thicknesses of the Si layers are indicated at the side of each layer. Close inspection of the TEM cross section shows that the shape of the adjacent interfaces are correlated only when the separation is below ~ 1.5 nm. We ascribe the vertical correlation observed here to the slow diffusion of the atoms on the sample surface during the crystal growth due to the low growth temperature of $\sim 300^\circ\text{C}$. The vertical correlation has been also observed in the multilayer arrays of coherently strained islands due to the resulting strain distribution.^{14,15} However, this mechanism does not apply to the present case since the composition and the strain of the Si and SiGe layers of the QC samples are rather uniform.

In summary, we analyzed the effect of the interface roughness on the broadening of the intersubband absorption and emission. We found a good agreement between the theory and the experiment for the diagonal and vertical intersubband transitions in $\text{GaInAs}/\text{AlInAs}$ structures. For the strain-compensated SiGe QCs, we compared the experiment

and the theory using the experimentally determined interface parameters and found that interface roughness limits the linewidth of the midinfrared EL. We found the importance of the vertical interface correlation on the interface-roughness-limited intersubband broadening for our SiGe QCs with thin layers below ~ 1.5 nm, leading to a partial cancellation of the interface roughness scattering effect.

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