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Piezoreflectance study of short-period strained Si-Ge superlattices grown on (001) Ge

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We have studied the stress-modulated reflectivity at 77 K of a series of short-period strained Si-Ge superlattices grown on (001) Ge substrates. These samples are similar (or identical) to those measured using electroreflectance (40 K) by Pearsall *et al.* [Phys. Rev. Lett. **63**, 2104 (1989)]. We have detected several low-energy features just above the direct band gap of Ge. The observed spacer-layer-thickness dependence of the transition energies and comparison to a calculation clearly show that they are due to quantum-confined direct transitions in the Ge spacer region, not pseudodirect transitions in the short-period Si-Ge portion of the samples.

The possibility of achieving pseudodirect optical transitions in the Si-Ge system through artificially ordered structures has recently received considerable experimental and theoretical attention.[1-3] Studies of valence-band offset and the well-known nature of the uniaxial strain in Si and Ge have established that the conduction-band edge in these structures is formed from ⟨100⟩-oriented Si states. Pseudomorphic, strained-layer epitaxy of a Si-Ge superlattice (SL) on a (001) Ge substrate creates a tensile, biaxial strain (in-plane), which results in a compression along the SL growth axis. Under these conditions of strain, the conduction-band edge lies along the SL axis, and it will be mixed by the SL potential with zone-center states. This effect raises the possibility that the SL might be a direct-gap material. Pearsall *et al.* have reported structure in the electroreflectance spectra at 40 K of such samples, which has been attributed to optical transitions at energies theoretically predicted for SL-induced direct optical transitions at the center of the Brillouin zone.[4,5] However, the interpretation of these results are complicated by the presence of Franz-Keldysh oscillations (FKO) whose origin are not clearly understood.[4,5]

We have investigated a number of short-period Si-Ge SL's grown on (001) Ge substrates, similar (or identical) to those of Refs. 4 and 5, using stress-modulated reflectivity [piezoreflectance (PzR)] at 77 K. Piezoreflectance also has proven to be a useful method for investigating semiconductor microstructures.[6] The observed spectra allow us to make an unambiguous assignment of the peaks since they do not exhibit FKO.[7] We find that the observed features just above the direct gap of Ge are clearly due to quantum-confined direct transitions in the Ge spacer regions, not pseudodirect transitions in the short-period Si-Ge portions of the sample as reported by Pearsall *et al.*[4,5]

The samples used in this study were grown by molecular-beam epitaxy[4,8] on (001) Ge substrates at 450 °C. One category had a unit cell consisting of three monolayers (ML) of Si and seven ML of $Ge(Si_3Ge_7)$, while the other had a unit cell of four ML of Si and six ML of $Ge(Si_4Ge_6)$. The samples alternated one of the above ordered unit cells, repeated 5 times, with pure Ge spacer regions of various thicknesses ranging from 29 to 143 ML. We designate such configurations as $(Si_mGe_n)_5Ge_N$, where N denotes the number of ML's of the Ge spacer. This overall pattern was repeated either 10 or 20 times. Two of the samples were from the same wafers used in Refs. 4 and 5. The periodic structure parameters were determined using high-resolution x-ray diffraction.[9] Stress modulation was achieved by mounting the samples on a 0.15-cm-thick zirconate-titanate piezoelectric transducer driven by a 500-V peak-to-peak sinusoidal wave at 1 kHz.[7]

Shown by the solid lines in Fig. 1 are the PzR spectra at 77 K of the (001) Ge substrate and four $(Si_mGe_n)_5Ge_N$

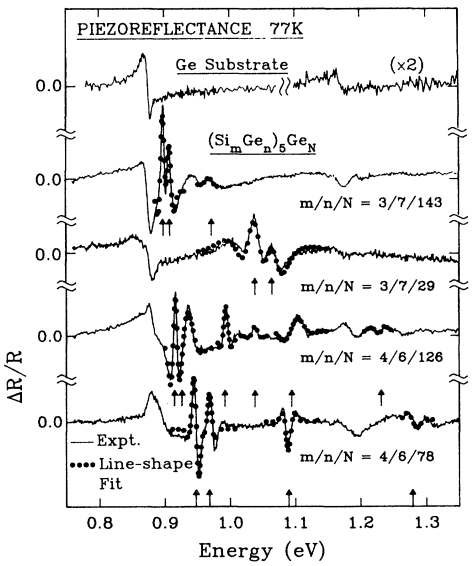

FIG. 1. Piezoreflectance spectra (solid lines) at 77 K of a (001) Ge substrate and $(Si_3Ge_7)_5Ge_{143}$, $(Si_3Ge_7)_5Ge_{29}$, $(Si_4Ge_6)_5Ge_{126}$, and $(Si_4Ge_6)_5Ge_{78}$ short-period SL samples. The dotted lines are least-squares fits to a FDGL function which yields the transition energies denoted by the arrows.

SL's with $m/n/N=3/7/143$, 3/7/29, 4/6/126, and 4/6/78. The sharp peak at 0.875 eV in the Ge substrate spectrum corresponds to the lowest direct gap (E_0) of this material while the weaker structure at 1.175 eV is due to the spin-orbit-split component ($E_0+\Delta_0$). The 3/7/143 and 4/6/126 samples, which are the same as Refs. 4 and 5, exhibit two well-resolved peaks just above the structure at 0.875 eV (which originates in the Ge substrate). The 3/7/29 and 4/6/78 materials also have doublets which are well separated from E_0. With decreasing N the doublets undergo a blueshift and the separation between the components increases. Except for the sample with the narrowest Ge spacer the other spectra exhibit a number of features above the doublet. The dotted lines are least-squares fits to a first-derivative Gaussian line shape (FDGL), which is appropriate for PzR at 77 K.[10] The obtained energies of the various peaks are denoted by arrows and also are listed in Table I.

The origin of the PzR peaks can be understood from the band diagram for the whole structure $(Si_mGe_n)_5Ge_N$, a point previously emphasized for similar structures grown in (001) Si substrates.[11] Self-consistent local-density-functional calculations have been performed for components of the full structure, e.g., the pure Ge, the Si_mGe_n SL or an alloy. These calculations[12] yield the necessary band extrema as well as band offsets. The eigenvalues from such calculations require self-energy corrections for both the bulk band gaps[13] as well as the valence-band offset.[14] These have been included approximately.[15] The band diagram shown in Fig. 2 for either a Si_4Ge_6 SL (solid lines) or the corresponding alloy (dotted lines), alternating with Ge, are a result of the above procedure.

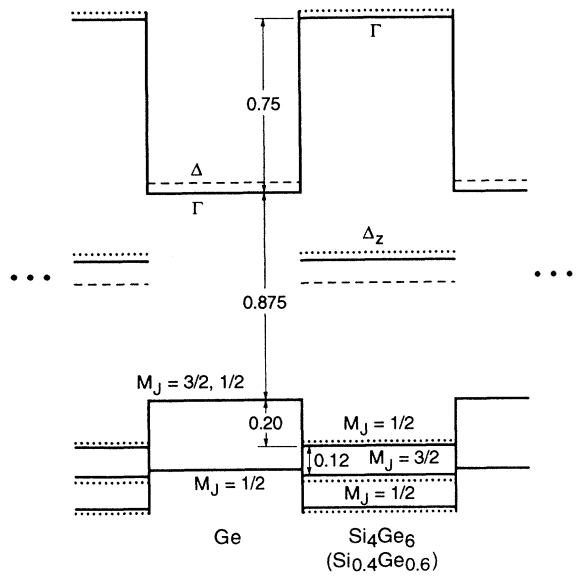

FIG. 2. Calculated band diagram for a superlattice alternating Ge spacer sections and the Si-Ge regions. The solid lines denote ordered Si_4Ge_6 portions, while the dotted lines show the corresponding alloy case. The dashed lines indicate indirect conduction-band minima. Only one Γ and Δ derived band extrema are shown. Energy separations are in eV.

TABLE I. Experimental and theoretical values of the transitions in short period $(Si_3Ge_7)_5$ and $(Si_4Ge_6)_5$ superlattices with different Ge spacer thicknesses.

	Experiment		Theory	
Superlattice	Ge spacer (ML)	Energy (eV)	Energy (eV)	Origin
$(Si_3Ge_7)_5$	143[a]	0.898	0.898	11*H*
		0.908	0.905	11*L*
		0.972	0.96	22*H*
			0.99	22*L*
			1.06	33*H*
			1.13	33*L*
	29	1.039	1.07	11*H*
		1.065	1.10	11*L*
$(Si_4Ge_6)_5$	126[a]	0.915	0.902	11*H*
		0.926	0.912	11*L*
		0.992	0.99	22*H*
		1.038	1.02	22*L*
		1.094	1.11	33*H*
		1.231	1.20	33*L*
	78	0.947	0.93	11*H*
		0.967	0.95	11*L*
		1.090	1.10	22*H*
			1.17	22*L*
		1.278	1.39	33*H*

[a]Same samples as Refs. 4 and 5.

Several salient features in Fig. 2 should be noted. First, in the present tetragonal symmetry (i.e., due to the strain), the relevant quantum number for the valence-band states is M_j only. There are two $M_j=\frac{1}{2}$ states in the Si-Ge region which couple to the light-hole and split-off states in the Ge. The $M_j=\frac{3}{2}$ state couples to the heavy-hole state in the Ge. Second, the lowest conduction bands in the ordered Si_4Ge_6 region are formed from zone-folded Δ_z states which are slightly split by the superlattice order. Only the second one couples to the *s*-like conduction-band state, but weakly as indicated by the small oscillator strength for direct transitions from the valence-band states. Note that while holes are confined in the Ge region, the lowest energy electrons are confined in the Si-Ge portion. This corresponds to the lowest optical transition. Third, the *s*-like Ge conduction-band states are confined by the corresponding states in the Si-Ge regions. These will give rise to strong dipole allowed transitions from the heavy- and light-holes confined in the Ge. Such transitions will dominate the observed optical response in the energy region immediately above the direct gap of the Ge (0.875 eV at 77 K). Fourth, the SL order has only a small influence on the band diagram. Therefore, the Si_3Ge_7 case was treated using an alloy approximation.

For direct comparison to experiment we have calculated the various subband energies using the envelope function method[16] and the band diagram of Fig. 2. In the Ge region we have used electron (*e*), light-hole (lh), and heavy-hole (hh) masses (in units of the free-electron

mass) of $m_e=0.038$, $m_{lh}=0.046$, and $m_{hh}=0.22$,[17] taken from experiment. In the Si_4Ge_6 region the masses along the z axis have been calculated to be $m_e=0.07$, $m_{v1}=0.09$, and $m_{v2}=0.24$, where $v1$ and $v2$ refer to the ground state $M_j=\frac{1}{2}$ and the $M_j=\frac{3}{2}$ valence states, respectively (see Fig. 2). Nonparabolicity effects have not been included. For the purposes of the subband calculation there is some ambiguity about the Ge well width since one of the Ge_n regions is contiguous to the Ge_N spacer. For the small N cases, or for higher subbands, this uncertainty of n ML of Ge in the well width alters the calculated confinement energies by as much as $\sim$50 meV, although the lh-hh splitting is much less affected. Therefore, the values reported represent an average. The final transition energies are the calculated confinement energies plus the measured bulk Ge transition energy of 0.875 eV taken from Fig. 1. The energies listed in Table I are "symmetry-allowed" confined transitions [$\alpha\alpha H(L)$] between the αth conduction to αth valence subband of heavy (H)- or light (L)- hole character. There is a distinct blueshift of all the features with decreasing N. Overall there is a very good agreement between experiment and theory. Thus, we can identify the various features in the PzR spectra with transitions in the quantum wells formed by the Ge spacer regions.

Pearsall *et al.* reported electroreflectance results at 40 K on $(Si_mGe_n)_5Ge_N$ SL's on (001) Ge with $m/n/N$ of 3/7/143 and 4/6/126. However, the spectra are complicated by strong FKO above E_0 and $E_0+\Delta_0$ of Ge. Thus, there is considerable ambiguity concerning the interpretation of features near E_0 and $E_0+\Delta_0$ as being due to SL-induced direct optical transitions. Also since these samples had a large N any features due to the Ge quantum well could also be masked by the FKO. Recently Menczigar *et al.*[18] have published photoreflectance results as a function of temperature on Si_mGe_n SL's grown on (001) Ge with $m/n=2/6$, 3/9, and 4/12. The authors interpret features in the 0.9–1.2 eV range for the 2/6 sample as being due to SL-induced direct interband transitions. However, their results also exhibit complex oscillating features above E_0 and $E_0+\Delta_0$ which complicates the analysis of the data.

In conclusion, we have investigated a number of $(Si_mGe_n)_5Ge_N$ SL's on (001) Ge using PzR at 77 K. Since the PzR spectra do not exhibit any FKO we have been able to make an unambiguous identification of the origins of the observed features. Based on the dependence on N and comparison with a theoretical calculation they are clearly due to direct transitions in the quantum well formed by the Ge spacer, not pseudodirect transitions in the short-period Si-Ge portion of the sample as reported in electromodulation experiments.

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