Direct Transition Energies in Strained Ten-Monolayer Ge/Si Superlattices

The $Ge_nSi_m(001)$ strained-layer superlattices (SLS's) with $n+m=10$ have received much attention[1,2] due to the possibility of obtaining quasidirect transitions. Using electroreflectance, Pearsall *et al.*[2] observed a peak at 0.96 eV in their Ge_6Si_4/Ge SLS's and assigned it to the direct transition between the heavy hole (hh) Γ_8^v and the zone-folded conduction-band minimum (CBM).

In a recent Letter, Zachai *et al.*[1] presented photoluminescence (PL) measurements of several ten-monolayer (ML) Ge_nSi_m SLS's. By far the strongest signal originated from the "symmetrically strained" Ge_4Si_6 superlattice (lateral strain in Si: $\epsilon_{\parallel}^{Si} \approx 1.4\%$) at 0.84 eV. They assigned it to the quasidirect gap. We believe that this interpretation—in disagreement with the results of Pearsall *et al.*[2]—is incorrect for the following reasons:

(a) We have performed extensive *ab initio* linear-muffin-tin-orbital (LMTO) band-structure calculations of 10-ML Ge_nSi_m SLS's which confirm that the 10-ML SLS's mentioned above are direct-gap materials. The error in the excitation energies introduced by the use of the local-density approximation has been corrected with "*ad hoc*" potentials placed at atomic sites, which yield the correct conduction bands and deformation potentials of the bulk materials Si and Ge.[3] We have transferred the correction parameters to the SLS's and obtain excellent agreement with the photoreflectance data of Pearsall *et al.*, for both their Ge_6Si_4/Ge (Ref. 2) and Ge_4Si_4/Si (Ref. 4) samples (see Table I). The differences between the experimental and calculated values are 0.03–0.07 eV, and thus lie almost within the experimental error. This strongly supports our estimate of the error in our calculation, which we rate to be at most 0.1 eV. The difference between our calculations and the PL results of Zachai *et al.*,[1] however, exceeds this error by a factor of 2–3.

(b) It is well known that dislocations in Si, Ge, and Ge_xSi_{1-x} alloys are electrically active and introduce local energy levels below the CBM. Weber and Alonso[5] found strong recombination radiation from misfit dislocations in $Ge_{0.4}Si_{0.6}$ alloys at about 0.84 eV (so-called D_2 band) in their PL experiments. This is exactly the energy at which the strongest luminescence was found in the Ge_4Si_6 SLS. Zachai *et al.* note that a "considerable amount of misfit dislocations"[1] exist in their SLS's. The weak polarization dependence (only 20% difference in the PL intensities of the two polarization geometries) was explained by the close energy separation of the hh and light hole (lh). Our calculations indicate this energy difference to be 0.04 eV, which should be observable.

TABLE I. Comparison of calculated and measured direct transitions. All energies are in eV.

	$\epsilon_{\parallel}^{Si}$ (%)	Experimental	LMTO	Identification
Ge_4Si_4	0.0	1.25[a]	1.29	hh: p_x,p_y
		1.70[a]	1.77	hh: p_x,p_y
Ge_6Si_4	4.2	Not observed	0.86	lh: p_z
		0.96[b]	0.99	hh: p_x,p_y
Ge_4Si_6	1.4	0.84[c]	1.08	hh: p_x,p_y
		0.84[c]	1.12	lh: p_z

[a]Electroreflectance, from Ref. 4.
[b]Electroreflectance, from Ref. 2.
[c]Photoluminescence, from Ref. 1 (see text).

The Kronig-Penney-type model described in Fig. 3 of Ref. 1 gives a hh-to-CBM direct transition for the Ge_6Si_4/Ge sample, which is about 0.2 eV lower than that measured by Pearsall *et al.*[2] Still, the values calculated with this simple model are about 0.1 eV higher than those measured in Ref. 1. These differences add up to the discrepancy of 0.2–0.3 eV which we find if we compare their PL experiments to our calculations.

In conclusion, we believe that the observed PL peak at 0.84 eV can be ascribed to recombination radiation from dislocations[6] or possibly other defects in the SLS's. The lowest direct transitions occur at about 1.1 eV.

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