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Optical absorption spectroscopy of Si-Ge alloys and superlattices

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We report calculations and measurements of the optical absorption coefficient of $\mathrm{Si}_n\mathrm{Ge}_m$ superlattices and alloys where $n \approx m$. Our results can be used to determine the fundamental band gap, the dependence of the band gap on superlattice period, and the absorption coefficient near the band-gap energy. Both theory and experiment show that all short-period ($n+m<20$) superlattices display a similar linear dependence of absorption coefficient on photon energy. This behavior is different from alloys of the same average composition where we measure that the absorption coefficient increases with the $\frac{3}{2}$ power of photon energy. [S0163-1829(96)02627-6]

Si-Ge semiconductors are being used to create high-performance bipolar transistors and integrated circuits,[1,2] highly integrated focal-plane array infrared detectors,[3] and infrared light-emitting diodes.[4] This progress demonstrates considerable promise for Si-based high-speed, low-power electronic and optoelectronic devices.[5,6] Numerous theoretical band-structure calculations of these Si-Ge superlattice structures have established that new band-edge states are formed at $\mathbf{k}=\mathbf{0}$ and that the optical matrix element between the top of the valence band and these new states is enhanced by several orders of magnitude over that of the optical matrix element for the lowest indirect transition. These calculations also show that the optical matrix element at $\mathbf{k}=\mathbf{0}$ remains at least one order of magnitude less than that observed in a direct gap semiconductor such as GaAs.[5]

In principle, the direct or indirect character of the fundamental band gap can be determined from the measurement of the optical absorption coefficient versus photon energy,

$$a(\hbar\omega)=\frac{4\pi^2\hbar c}{V}\int W(E)\mathcal{N}(E)dE, \qquad (1)$$

where $W(E)$ is the transition probability and $\mathcal{N}(E)$ is the density of states.[7] In a direct-gap material, each state in the valence band is connected with one state in the conduction band because $\mathbf{k}_f-\mathbf{k}_i=0$, leading to simple integration of Eq. (1). In the case of an indirect-gap material, $\mathbf{k}_f$ is connected by the phonon momentum $\mathbf{k}_p$ to a multiplicity of initial states leading to a different dependence of the optical absorption coefficient on energy, when Eq. (1) is integrated:

$$\alpha(\hbar\omega)=A(\hbar\omega-E_g)^{1/2} \quad \text{(direct band gap)}, \qquad (2)$$

$$a(\hbar\omega)=B(\hbar\omega-E_g)^{2} \quad \text{(indirect band gap)}. \qquad (3)$$

Equation (2) can be applied to the study of GaAs or InP, while Eq. (3) applies to Si and Si-Ge random alloy materials. However, neither equation can be applied to Si-Ge short-period superlattices. The near-edge band structure of the conduction band does not satisfy the basic simplifying assumptions leading to Eqs. (2) and (3).

The near-edge valence-band structure of a Si-Ge short-period superlattice still resembles that of Si or GaAs. While the superlattice potential will cause zone folding of the band structure to occur, the new states lie at energies of several hundred meV below the top of the valence band. Hence they do not play a role in our experiments. However, the same situation does not hold for the conduction band. Here the effect of zone folding is to produce several nearly degenerate states at the band edge. The E-$\mathbf{k}$ relationship for these states is not parabolic over an energy range comparable to a phonon energy and hence there is no longer a simple expression for the dependence of the density of states on energy. However, Eq. (1) is still valid, that is, the optical absorption coefficient has the same dependence on photon energy as has the density of states. As a result, the functional form of the absorption coefficient can be expressed

$$a(\hbar\omega)=C(\hbar\omega-E_g)^{x}, \qquad (4)$$

where x is to be determined. We have measured the optical absorption coefficient and its dependence on photon energy. In order to compare these results to theory, it is necessary to calculate the density of states from the actual band structure of the specific superlattices that we are measuring. Once the density of states (in numerical form) is known, the optical absorption coefficient can be calculated. In this paper we report the results of this measurement and calculation.

The theoretical determination of the absorption coefficient was achieved using an empirical tight-binding method that has been adjusted to give excellent agreement for the optical properties of bulk Si and Ge.[8] The basis set uses sp^3 orbitals

TABLE I. Summary of sample structures measured in this work.

Sample	Type	Composition	Superlattice Thickness (nm)	Band gap (eV)	Buffer Composition	Buffer Thickness (nm)	Cap Composition	Cap Thickness (nm)	Substrate Doping
B2211	Alloy	$Si_{0.5}Ge_{0.5}$	263	0.76	$Si_{0.25}$	20	Si	1	$p^{-}<10^{14}$
B2208		5:4	270	0.71	$Si_{0.25}$	20	Si	1	$p^{-}<10^{14}$
B2209		6:5	277	0.70	$Si_{0.25}$	20	Si	1	$p^{-}<10^{14}$
B2210		7:6	313	0.65	$Si_{0.25}$	20	Si	1	$p^{-}<10^{14}$

with spin-orbit coupling included. The method has been tested successfully by calculation of the deformation potentials and optical properties of Si-Ge superlattices.[4] The absorption coefficient depends mainly on the joint density of states that is deduced directly from the band structure. We have considered only direct interband transitions to determine the absorption coefficient. This procedure tends to underestimate the absolute magnitude of the absorption coefficient by ignoring the contribution from indirect transitions, which may be substantial in short-period superlattice materials such as these. A most important aspect of the calculation is that the optical properties are integrals over the Brillouin zone and an appropriate integration method should be selected. In the present case we have used the very successful linear analytic tetrahedron method.

All superlattices were grown by MBE symmetrically strained along the (001) direction on Si substrates. The superlattices are continuous alternating sections of n layers of Si and m layers of Ge whose thicknesses vary between 2500 and 3200 Å depending on the sample. Following growth, these samples have been extensively characterized to determine composition, periodicity, and strain. It was our intent to study superlattices with periods of 4 ML of Si and 4 ML of Ge (4:4), (5:5), and (6:6). In this way the average composition would be the same as that of a $Si_{0.5}Ge_{0.5}$ alloy. However, the actual periods of these superlattices are slightly different. A more detailed description of the samples is given in Table I. These superlattices and alloys all have the important feature that the thickness of the buffer layer between the superlattice and the substrate is much less than the thickness of the superlattice itself. The samples were prepared for measurement by etching away the superlattice on a portion of each sample so that the substrate was exposed.

Absorption measurements were made using direct differential comparison between the optical transmission of the substrate alone and substrate plus superlattice combination. The absorption coefficient was extracted from the data using Beer's law. Additional details of this experimental technique have been described in earlier work by us and others.[9–12]

Our experimental results are shown in Figs. 1–3. The absorption coefficient is plotted versus the phonon energy–band-gap energy. Data can be taken over a range of photon energy from the infrared ($\hbar\omega = 0.5$ eV) to the onset of absorption by the Si substrate ($\hbar\omega = 1.0$ eV). The band gap was determined from the data as the highest energy at which there was no measurable difference between the optical transmission through the substrate and the optical transmission through the combination of the substrate and superlattice. The band-gap energy is given both in the figures and in Table I. The experimental data in Figs. 1–3 are plotted in log-log form. The slope of the data gives the power-law dependence x that describes the relationship between the absorption coefficient and the photon energy. In Fig. 1 we show the measured absorption coefficient for the $Si_{0.5}Ge_{0.5}$ pseudorandom alloy. The band gap is 0.76 eV. The absorption coefficient depends on the $\frac{3}{2}$ power of the photon energy. In Fig. 2(a) we show the measured absorption coefficient for a Si-Ge (5:4) superlattice. In Figs. 2(b) and 2(c) we show the result of calculations. The absorption coefficient depends linearly on the photon energy for the measurement. The result is less clear for the calculations. However, the measured values for the absorption coefficient are about two orders of magnitude larger than the calculated results. The band gap obtained from the measurement is 0.71 eV, while the calculated values are larger. In Fig. 3(a) we show the results of our measurement on a Si-Ge (6:5) short-period superlattice and compare this result to theory in Fig. 3(b). Once again the absorption coefficient is seen to show a linear dependence on photon energy. In Fig. 3(b) the calculated absorption coefficient is displayed using the same procedure as for the experimental results in order to facilitate direct comparison. The calculated absorption coefficient depends nearly linearly on the photon energy near the band edge $0.01 < (\hbar\omega - E_g) < 0.10$ eV, where theory can be compared to experiment.

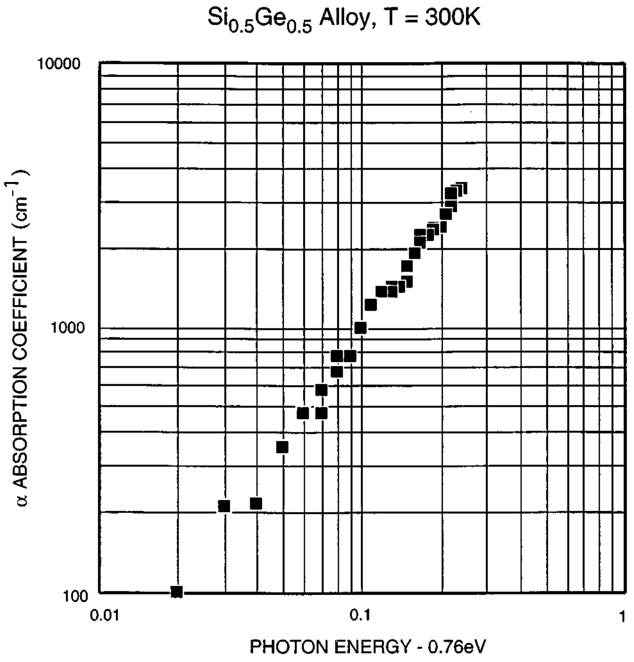

FIG. 1. Optical absorption coefficient versus photon energy for a $Si_{0.5}Ge_{0.5}$ pseudorandom alloy. Data are taken at 300 K by optical transmission spectroscopy. The slope of the log-log plot gives the exponent relating the absorption coefficient to the photon energy. In the case of this alloy, this exponent can be seen by these data to be $\frac{3}{2}$.

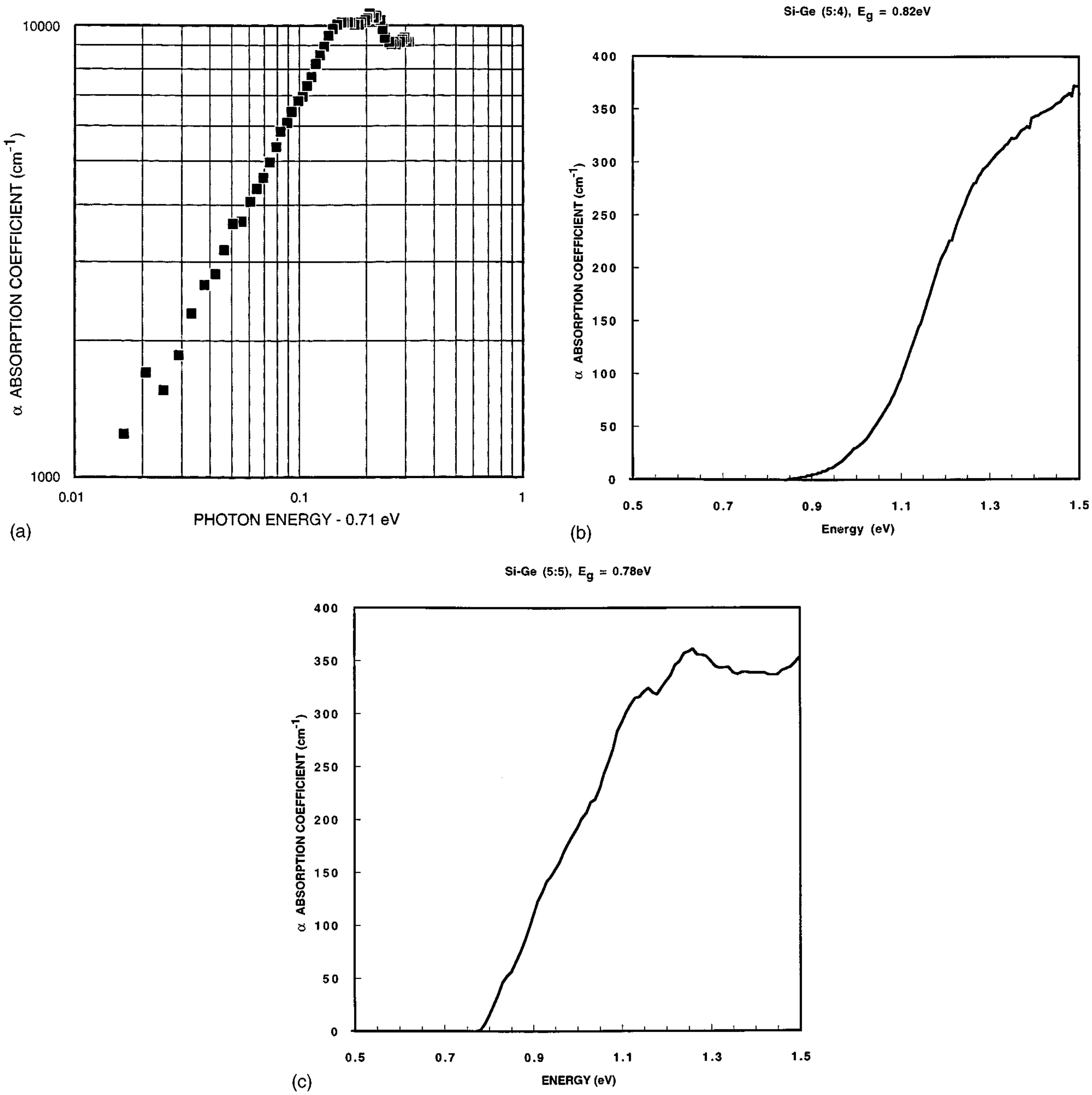

FIG. 2. Optical absorption coefficient: comparison of experiment with theory. (a) Optical absorption coefficient of a Si-Ge (5:4) superlattice taken at 300 K by optical transmission spectroscopy. The absorption coefficient is seen to vary linearly with the photon energy above the band gap of 0.71 eV, which is also determined by this measurement. (b) Calculated absorption coefficient for a Si-Ge (5:4) superlattice versus photon energy. To compare experiment with theory, the data would correspond to the range of 0.85–1.05 eV on this curve. In this range, the dependence of the calculated absorption coefficient on photon energy is exponential with $x>1$. (c) Calculated absorption coefficient for a Si-Ge (5:5) superlattice versus photon energy. To compare experiment with theory, the data would correspond to the range of 0.8–1.0 eV on this curve. In this range, the dependence of the calculated absorption coefficient on photon energy is linear, in agreement with experiment.

Here it can be seen that the experiment values for the absorption coefficient lie about two orders of magnitude above calculated values. A similar comparison can be made for a Si-Ge (7:6) superlattice that has a measured band gap of 0.65 eV. Optical absorption measurements on two additional short-period superlattices show the same linear dependence.

The following trends are seen in the experimental data: (i) the absorption coefficient depends linearly on the photon energy for superlattices, (ii) the absorption coefficient depends on the $\frac{3}{2}$ power for the alloy of the similar average composition, (iii) the magnitude of the measured absorption coefficient is larger than theory predicts for the superlattices, and (iv) the measured band gap increases as the superlattice period decreases, with the alloy having the largest band gap. The power dependence describing the relationship between absorption coefficient and photon energy for the superlattices that we obtain from this measurement (i.e., $x=1$) is different from that obtained by Olajos *et al.* in photoconductivity studies (e.g., $x=2$).[12] Our photoconductivity spectra show a nonlinear dependence of photocurrent on the photon energy near the band edge, in good agreement with the work of Olajos *et al.* Our work so far demonstrates that optical transmission

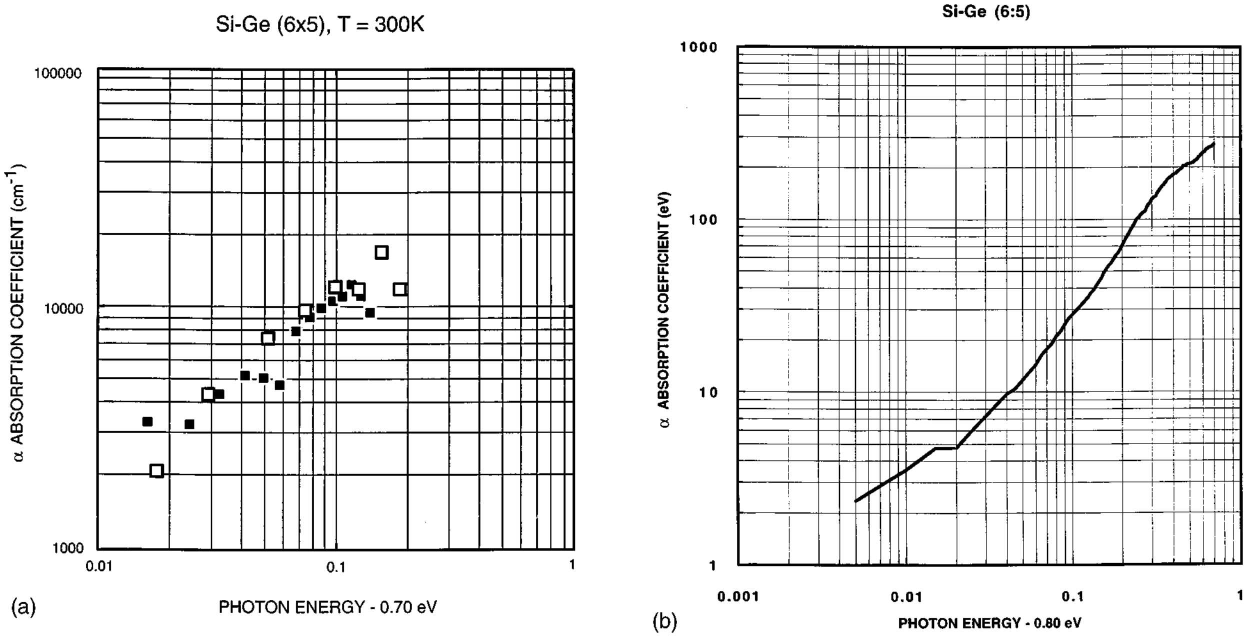

FIG. 3. Optical absorption coefficient: comparison of experiment with theory. (a) Optical absorption coefficient of a Si-Ge (6:5) superlattice taken at 300 K by optical transmission spectroscopy. Data are shown from two samples cut from the same wafer. The absorption coefficient is seen to vary linearly with the photon energy above the band gap of 0.70 eV, which is also determined by this measurement. (b) Calculated absorption coefficient for a Si-Ge (6:5) superlattice versus photon energy. We have displayed the calculated data in the same form as the experiment for direct comparison. Both the experimental data and the calculated absorption show a linear dependence on photon energy. The measured absorption coefficient is about 300 times larger than the calculated value.

spectroscopy and photocurrent spectroscopy measurements are not equivalent. Similar differences have been noted by Schrottke *et al.* in their study of GaAs/Al$_x$Ga$_{1-x}$As superlattices.[13]

For all the superlattice samples that we have measured in this study, the absorption coefficient depends linearly on photon energy. Theory shows that this result is expected because of the large number of conduction-band states that lie close to the band-gap energy throughout the Brillouin zone. Band-to-band absorption contains both direct and indirect contributions. The energy dependence does not follow simple analysis, but derives its energy dependence from the joint density of states. These results show that short period superlattices do produce a new synthetic three-dimensional band structure. The experimentally measured band gap is found to be about 20% lower than that determined by theory. This effect may be the result of absorption by localized band-edge states formed by dislocations of defects in the sample. The experimentally measured absorption coefficient is several orders of magnitude larger than that calculated by theory near the band edge. Finally, the dependence of optical absorption on photon energy, while in good agreement with theory, does not agree with the energy dependence of the photoconductive response in the same samples over the same energy range. These differences indicate that the physics of band-to-band transitions in Si-Ge superlattices is not completely understood. We are currently pursuing research to clarify these issues.

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