Admittance spectroscopy measurements of band offsets in $Si/Si_{1-x}Ge_x/Si$ heterostructures

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Admittance spectroscopy has been used to measure conduction- and valence-band discontinuities in $Si/Si_{1-x}Ge_x$ heterojunctions ($0<x<0.45$). Most of the band-gap discontinuity was in the valence band. The measured valence-band offset increased with increasing Ge concentration in the strained $Si_{1-x}Ge_x$ films, and it decreased when the $Si_{1-x}Ge_x$ layers started to relax. These results indicate that admittance spectroscopy can be used to monitor the electronic properties of transistorlike $Si/Si_{1-x}Ge_x/Si$ heterostructures.

The successful use of epitaxial $Si_{1-x}Ge_x$ layers to fabricate silicon-based heterojunction bipolar transistors[1,2] has created considerable interest in the electronic properties of $Si/Si_{1-x}Ge_x$ heterostructures. Since band discontinuities are among the critical parameters determining device performance, a great deal of effort has been focused on determining their values. Theoretical calculations[3,4] and experimental data obtained from photocurrent spectroscopy,[5] x-ray photoelectron spectroscopy,[6] and transistor measurements[7] demonstrated that most of the band-gap difference between a strained $Si_{1-x}Ge_x$ layer and an unstrained Si substrate appeared as a valence-band offset. In this letter we present admittance spectroscopy measurements[8–10] of the conduction- and valence-band discontinuities in a transistorlike structure consisting of a single, thin, strained $Si_{1-x}Ge_x$ layer sandwiched between thick Si layers. These transport measurements in such a structure allow independent determination of the band discontinuities with high accuracy.

The samples for this study were epitaxially grown by the chemical-vapor-deposition technique (limited reaction processing[11]) on (100)-oriented Si substrates. Each sample contained three epitaxial layers: a 2-μm-thick Si buffer layer on the Si substrate, a 30-nm-thick $Si_{1-x}Ge_x$ layer, and a Si cap with thickness between 0.2 and 0.4 μm. The Ge content in the $Si_{1-x}Ge_x$ layer was varied between 10% and 45%, and was constant throughout the thickness of each $Si_{1-x}Ge_x$ layer. All epitaxially grown layers in one sample were either n type (As doped, grown on n^+ substrates) or p type (B doped, grown on p^+ substrates) with dopant concentrations ranging from 10^{16} to 10^{17} cm^{-3}. The $Si_{1-x}Ge_x$ layers were typically doped 2–5 times more heavily than the adjacent Si layers. Junctions required for electrical measurements were formed by shallow As implants into the p-type Si caps or by depositing Schottky diodes on the n-type Si caps. Ohmic contacts were fabricated on the back sides of the wafers. Dopant concentrations and layer thicknesses were determined from capacitance-voltage measurements and secondary-ion mass spectroscopy (SIMS) profiling. Ge profiles were measured using SIMS. Ge contents were also determined in corresponding $Si_{1-x}Ge_x/Si$ layers without Si caps using SIMS and Rutherford backscattering (RBS). The band offsets are affected by the strain in $Si_{1-x}Ge_x/Si$ layers. The strain and misfit dislocation structure have been previously determined in similar layers by x-ray diffraction, x-ray topography, and transmission electron microscopy.[12,13]

Figure 1 shows a partial band diagram of the experimental samples. Capacitance-voltage measurements confirmed that the $Si_{1-x}Ge_x$ layer remained outside the depletion region of the junction. Following Letarle *et al.*,[10] the equivalent circuit of the sample (Fig. 1) consists of a depletion layer capacitance C_d, and the capacitance C_u and conductance G_u of the undepleted region. Admittance spectroscopy consists of measuring the ac capacitance and conductance as a function of temperature at various frequencies.[14] It is assumed[9,10,15] that the conductance can be expressed in terms of thermionic emission across the potential barrier caused by the band offset between the Si and $Si_{1-x}Ge_x$. This assumption requires that only a negligible number of traps are present in the Si and the $Si_{1-x}Ge_x$ so that the signal originating from the carriers crossing the band offset is not perturbed by the thermal emission of carriers from the traps. Deep-level transient spectroscopy (DLTS), combined with temperature-dependent capacitance-voltage measurements of similarly grown Si and $Si_{1-x}Ge_x$ layers,[16] showed that the Si layers were free of deep states and that only an insignificant ($<5\times10^{11}$ cm^{-3}) number of traps was present in the $Si_{1-x}Ge_x$. The resonant frequency f_T of the equivalent circuit is equal to $f_T=G_u/2\pi(C_d+C_u)$. The conductance G, corresponding to thermionic emission across the band discontinuity, can be expressed[9,10] as

$$G=\frac{q^2Sv_{\rm th}(T)N_v(T)}{kT}\exp\left(-\frac{\Delta E+E_F}{kT}\right)$$
$$=\alpha kT\exp\left(-\frac{\Delta E+E_F}{kT}\right), \quad (1)$$

where q is the electron charge, S is the device area, $v_{\rm th}$ is the

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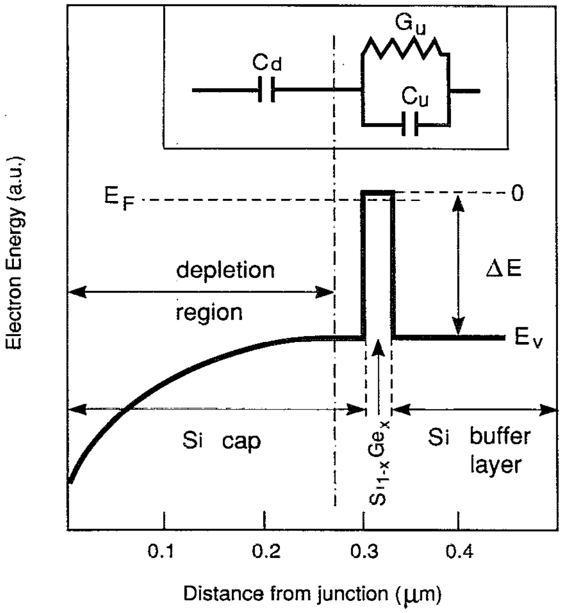

FIG. 1. Valence-band diagram of a junction on p-type $Si/Si_{1-x}Ge_x/Si$ heterostructure. Insert shows the electrical equivalent circuit.

thermal velocity of the carriers, N_v is the effective density of states in the valence band, k is Boltzmann constant, T is the temperature, E_F is the Fermi level, ΔE is the valence-band discontinuity, and α is a temperature-independent constant in the temperature range of the present experiment. Figure 2 shows the peak in the measured parallel conductance and the step in the parallel capacitance from which the resonant frequency f_T is found. An Arrhenius plot of f_T/kT as a function of inverse temperature gives the activation energy E_a, which is then used along with Eq. (1) to calculate the band offset.

Admittance spectroscopy measurements were conducted over the temperature range from 90 to 300 K, under reverse bias of either 0 or 1 V, and at frequencies ranging from 100 Hz to 10 MHz. Measured values of the activation energy E_a were then used in Eq. (2) in order to obtain the valence-band offset values[9,10] for various Ge fractions:

$$\Delta E = E_a - E_F + |E_1| + kT \ln \alpha + \delta, \tag{2}$$

where E_1 is the lowest allowed energy level in the $Si_{1-x}Ge_x$ quantum well, and δ is the barrier lowering caused by thermally assisted tunneling across the barrier at the $Si_{1-x}Ge_x/Si$ boundary. E_1 was calculated assuming depth of the quantum well given by the theoretical band discontinuity calculations[3,4] including parabolic distortion of the bottom of the well caused by carrier redistribution into the well. Its value never exceeded 6 meV. The effective mass m^* values were calculated using the linear interpolation between Si and Ge values, and taking into account strain-induced band splitting.[3,4,17] E_F was calculated at 0 K by taking the ratio of the two-dimensional carrier density (assumed equal to the dopant concentration in the well times the width of the well) and the two-dimensional density of states $4\pi m^*/h^2$. E_F was assumed not to vary with temperature; it was estimated[10] that the error introduced by this assumption did not exceed 10 meV. Calculations of the prefactor α included changes in the valence-band structure caused by a biaxial compressive strain in the $Si_{1-x}Ge_x$.[3,4,17] δ was calculated as previously proposed;[18] it was found to be less than 3 meV and was therefore neglected in the calculations. The conduction-band offset values were calculated similarly.

Figure 3 presents measurements of the band offsets for both conduction and valence bands. As expected, most of the band-gap discontinuity is in the valence band. The con-

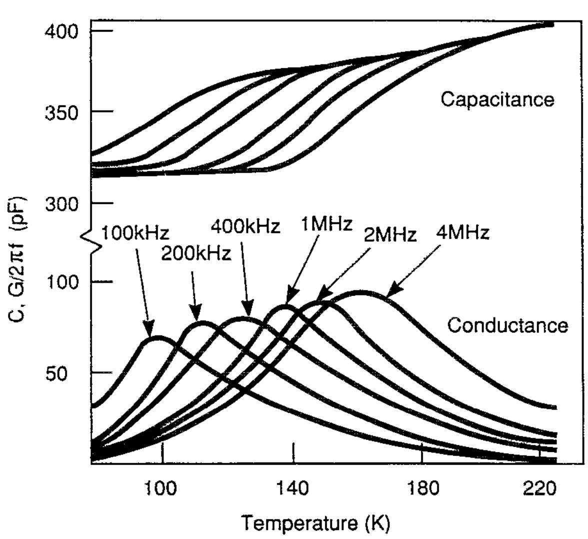

FIG. 2. Capacitance and conductance of the $Si/Si_{0.7}Ge_{0.3}/Si$ heterostructure as a function of temperature for various frequencies measured under zero-bias conditions.

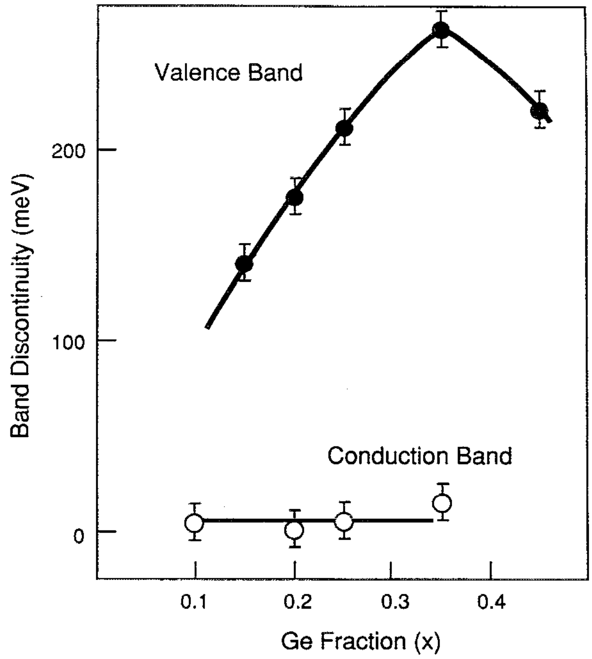

FIG. 3. Conduction- and valence-band offsets in $Si/Si_{1-x}Ge_x/Si$ heterostructures with corresponding error bars measured for Ge fractions (x) ranging from 0.1 to 0.45.

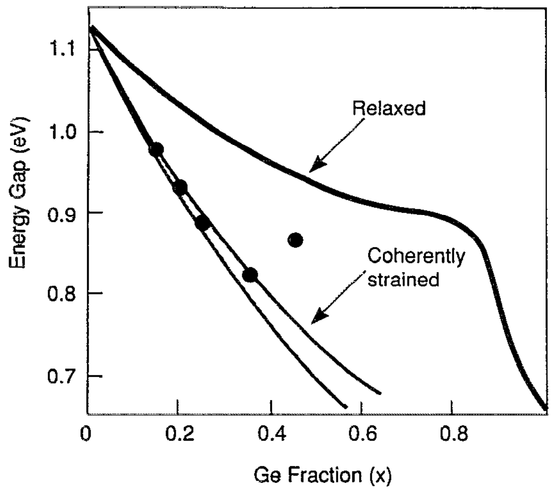

FIG. 4. Measured energy gap compared to theoretical band-gap calculations for coherently strained (Ref. 3) and relaxed (Ref. 19) $Si_{1-x}Ge_x$ layers at 300 K.

duction-band offset is of the order of several meV and is comparable to the experimental error. The decrease in the valence-band offset when $x > 0.4$ is most likely due to strain relaxation. From previous experiments[12,13] onset of the relaxation in the 30-nm-thick, capped $Si_{1-x}Ge_x$ layers should occur between $x = 0.35$ and $x = 0.4$. This interpretation is further illustrated in Fig. 4, where the experimental points are superimposed on plots of the band gaps of coherently strained[3] and unstrained[19] $Si_{1-x}Ge_x$ at the temperature of 300 K. It is assumed that all of the band-gap discontinuity occurs in the valence band, and the experimental data are adjusted using the temperature coefficient of the Si indirect band gap.[20]

In conclusion, conduction- and valence-band discontinuities between strained or partially relaxed $Si_{1-x}Ge_x$ and Si were measured by admittance spectroscopy. The results obtained are in good agreement with previous theoretical and experimental data, indicating that almost all of the band-gap discontinuity occurs in the valence band. Measurements were conducted on transistorlike heterostructures, demonstrating that admittance spectroscopy can be used for routine monitoring of electronic properties of $Si/Si_{1-x}Ge_x/Si$ heterostructures.

[1] T. I. Kamins, K. Nauka, J. B. Kruger, J. L. Hoyt, C. A. King, D. B. Noble, C. M. Gronet, and J. F. Gibbons, IEEE Electron. Device Lett. **10**, 503 (1989).

[2] G. L. Patton, J. H. Comfort, B. S. Meyerson, E. F. Crabbe, G. J. Scilla, E. de Fresart, J. M. C. Stork, J. Y.-C. Sun, D. L. Harame, and J. N. Burghartz, IEEE Electron. Device Lett. **11**, 171 (1990).

[3] R. People, Phys. Rev. B **32**, 1405 (1985).

[4] C. G. Van de Walle and R. M. Martin, Phys. Rev. B **34**, 5621 (1986).

[5] D. V. Lang, R. People, J. C. Bean, and A. M. Sergent, Appl. Phys. Lett. **47**, 1333 (1985).

[6] W.-X. Ni, J. Knall, and G. V. Hansson, Phys. Rev. B **36**, 7744 (1987).

[7] C. A. King, J. L. Hoyt, and J. F. Gibbons, IEEE Trans. Electron. Devices **ED-26**, 2093 (1989).

[8] D. V. Lang, M. B. Panish, F. Capasso, J. Allam, R. A. Hamm, A. M. Sergent, and W. T. Tsang, Appl. Phys. Lett. **50**, 736 (1987).

[9] R. E. Cavicchi, D. V. Lang, D. Gershoni, A. M. Sergent, J. M. Vandenberg, S. N. G. Chu, and M. B. Panish, Appl. Phys. Lett. **54**, 739 (1989).

[10] X. Letarle, D. Stievenard, M. Lannoo, and D. Lippens, J. Appl. Phys. **68**, 116 (1990).

[11] J. F. Gibbons, C. M. Gronet, and K. E. Williams, Appl. Phys. Lett. **47**, 721 (1985).

[12] M. P. Scott, S. S. Laderman, T. I. Kamins, S. J. Rosner, K. Nauka, D. B. Noble, J. L. Hoyt, C. A. King, C. M. Gronet, and J. F. Gibbons, Mater. Res. Soc. Symp. **130**, 179 (1989).

[13] D. B. Noble, Ph. D. thesis, Stanford University, 1991.

[14] D. L. Losee, J. Appl. Phys. **46**, 2204 (1975).

[15] J. Batey, S. M. Wright, and D. J. DiMaria, J. Appl. Phys. **57**, 484 (1985).

[16] K. Nauka, S. S. Laderman, S. J. Rosner, T. I. Kamins, M. P. Scott, C. A. King, J. L. Hoyt, and J. F. Gibbons, Bull. Am. Phys. Soc. **35**, 416 (1990).

[17] E. P. O'Reilly, Semicond. Sci. Technol. **4**, 121 (1989).

[18] D. V. Lang, in *Heterojunction Band Offsets*, edited by F. Capasso and G. Margaritondo (North-Holland, Amsterdam, 1989), pp. 377–396.

[19] R. Braunstein, A. R. Moore, and F. Herman, Phys. Rev. **109**, 695 (1958).

[20] See Landolt-Bornstein, *Numerical Data and Functional Relationships in Science and Technology, Physics of Group IV Elements and III-V Compounds*, edited by O. Madelung (Springer, New York, 1982), Vol. 17a, p. 43.