Charged carrier transport in $Si_{1-x}Ge_x$ pseudomorphic alloys matched to Si—strain-related transport improvements

J. M. Hinckley, V. Sankaran, and J. Singh
Center for High Frequency Microelectronics, Department of Electrical Engineering and Computer Science, The University of Michigan, Ann Arbor, Michigan 48109-2122

(Received 17 April 1989; accepted for publication 28 August 1989)

Charge carrier transport studies are reported for $Si_{1-x}Ge_x$ pseudomorphic alloy layers matched to the (001) Si substrate lattice constant. The effect of biaxial compressive strain on transport is studied by first examining the band structure changes via deformation potential theory and then studying the transport via a generalized Monte Carlo approach. Marked improvements in in-plane hole transport are obtained while significant improvements also occur in the out-of-plane electron transport. These changes are ideally suited for use in n(Si)-p($Si_{1-x}Ge_x$)-n(Si) heterojunction bipolar transistors.

Band-edge degeneracies in semiconductors are a key reason for poor transport because of the large angle scatterings involved in most interband transitions together with a large phase space available for scattering. Thus the improved electron transport in GaAs compared to Si is primarily due to the band edge being singly degenerate (Γ point) in GaAs and sixfold degenerate (near X point) in Si. Similarly, most semiconductors have poor hole transport due to light hole (LH), heavy hole (HH) degeneracy. In Si, the situation is worsened because of the very small spin orbit splitting separating the split-off (SO) band.

New developments in growth of pseudomorphic (i.e., the in-plane lattice constant is the same as the substrate) lattice-mismatched films provide a viable way to lift band-edge degeneracies. Improved p-type modulation-doped field-effect transistors (MODFETs),[1–4] enhanced optical device performance,[5] and improved strained base heterojunction bipolar transistors (HBTs) using Si Ge systems[6–10] have been reported. Perhaps the Si-SiGe system stands most to benefit from those developments due both to the potential of heterostructure concepts being available in Si technology and to improvements in transport properties in the alloy. Basic transport studies in the strained SiGe system are essential for device design and projection of device potential. No such studies currently exist.

In this letter we present results for hole and electron Monte Carlo transport calculations in $Si_{1-x}Ge_x$ pseudomorphic alloy layers. The general problem of transport in semiconductors involves calculating the scattering rates for various scattering mechanisms. According to the Fermi golden rule, the scattering rate is

$$W(\mathbf{k}) = \frac{V_c}{(2\pi)^3}\frac{2\pi}{\hbar}\int d^3k'|M(\mathbf{k},\mathbf{k}')|^2\delta(E+\Delta E-E') = \int d\Omega'\frac{dW(\mathbf{k},\mathbf{k}')}{d\Omega'}, \quad (1)$$

where $d^3k' = d\Omega' k'^2 dk'$. M is the scattering matrix element for the given scattering process, V_c is the crystal volume, and the density of final states is given by the δ function. The differential scattering rate $dW(\mathbf{k},\mathbf{k}')/d\Omega'$ is proportional to the post-scattering state probability distribution. The matrix elements $M(\mathbf{k},\mathbf{k}')$ for the modeled scattering mechanisms (e.g., phonons, interband scattering and intraband scattering, alloy scattering) are well known. Monte Carlo methods for calculating transport properties once the scattering rates and their angular distributions are known are well documented. The main change required in applying the Monte Carlo methods to the strained system is accounting for the complex nature of the band structure, which requires the numerical evaluation of the scattering rates.

Theoretical analysis of hole transport is more complicated than that of electron transport. This is primarily due to the strong coupling of the heavy, light, and split-off hole valence bands, which in the absence of spin orbit coupling, are degenerate at $\mathbf{k}=0$ and have the symmetry of the Γ_{25}' representation. Materials such as silicon and high silicon content alloys, which have a small spin orbit splitting, retain a high degree of coupling between all three valence bands. This coupling leads to strong warping of the constant energy surfaces. Usually, comparatively simple analytical expressions are used to represent the overlap function part of the scattering matrix element.[11–13] However, in the SiGe system, the usual simplifications cannot be made for p-type transport. Furthermore, strain induces changes not only in the band structure, but in the valence-band electronic states, requiring direct solution of the eigenstates from a 6×6 valence-band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian matrix. In our calculations, we retain the full band structure of the hole states and explicitly evaluate the matrix element for scattering as a function of initial and final wave vectors separately. This of course increases the complexity of our calculations.[14]

The hole transport studies are based upon (i) identifying the band structure changes in the valence band via a $\mathbf{k}\cdot\mathbf{p}$ calculation (including HH, LH, and SO bands) and a valence-band deformation potential theory, (ii) numerical calculations of the post-scattering state probability distributions and scattering rates for acoustic phonons,[15] nonpolar optical phonons (Si-Si like and Ge-Ge like), and alloy scattering,[16] (iii) a full Monte Carlo high-field simulation to calculate the carrier properties. In this letter we report results for undoped material; extrinsic effects associated with the Si-Ge optical phonon have been neglected. Harrison and Hauser's model for alloy scattering,[16] which we use in this work, is characterized by a spherically symmetric square well scattering potential of depth U_0. We have investigated

 0003-6951/89/452008-03$01.00

hole transport as a function of U_0 from 0.0 to 0.4 eV, and find a small monotonic decrease in carrier velocity with increased U_0. In the absence of experimental data to guide the choice of an effective alloy scattering potential, U_0, we have taken $U_0 = 0.2$ eV in the present work. This is on the order of half of the band-gap discontinuity between Si and Ge. Electron transport is essentially studied in the same manner, except the problem is much more simplified due to the analytic nature of the scattering rates. As a check on our formalism, we compare our results with published experimental results in Si and Ge (circles and triangles: Ref. 17; squares: Ref. 18).

In Figs. 1(a) and 1(b) we show a comparison of the hole E-k diagram for Si and $Si_{0.6}Ge_{0.4}$, respectively. The alloy has 1.56% in-plane lattice mismatch with respect to Si, and the compressive strain is reflected in the HH-LH and HH-SO band splittings. Figure 1(c) shows the splittings in the conduction and valence bands, as a function of Ge fraction in the alloy. The lifting of degeneracies due to strain has a very strong effect on both the electron and hole transport properties. This is because carriers in the strained system will be required to overcome an energy threshold, corresponding to the splittings, before interband transitions can occur.

In Fig. 2(a) we show the calculated in-plane (along [100] direction if growth is along (001) direction) hole velocity-field relationships for Si and Si-Ge alloys. The results are for 10% step increases in Ge content from Si ($x = 0$) to $Si_{0.6}Ge_{0.4}$ ($x = 0.4$). Also shown are experimental points reported in the literature for Si and Ge. Agreement with the published data provides confidence in our formalism. There is a steady improvement in the carrier transport, both at low fields and high fields, as the strain increases. However, the advantages to transport in increased Ge content alloys are

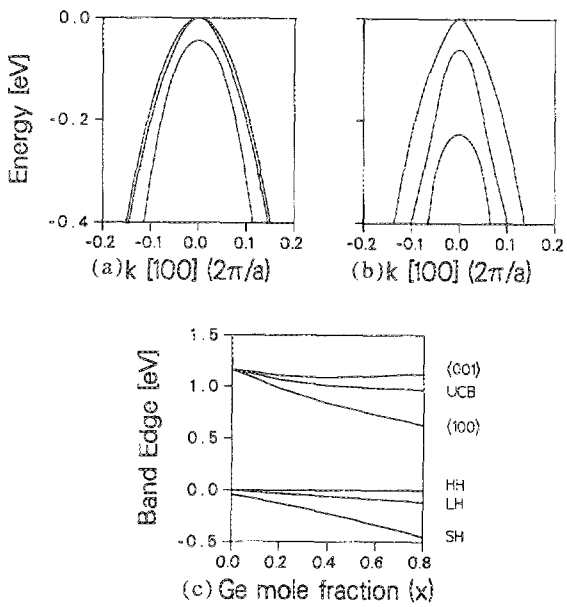

FIG. 1. Hole dispersion curves for (a) Si and (b) $Si_{0.6}Ge_{0.4}$; (c) splittings of the conduction band and valence band are shown as a function of alloy composition. UCB: unstrained conduction band, ⟨001⟩: out-of-plane X valleys, ⟨100⟩: in-plane X valleys, HH: heavy hole band, LH: light hole band, SH: split-off band.

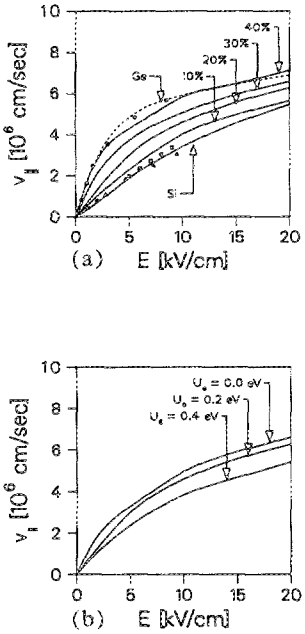

FIG. 2. (a) Calculated in-plane (along [100]) hole velocity field results for Si and $Si_{1-x}Ge_x$ alloys (with x increasing in steps of 0.1), experimental points are shown for Si and Ge; (b) effect of alloy scattering potential on transport properties.

tempered by a decreased critical thickness in such materials. Figure 2(b) shows the effect of the choice of alloy scattering potential on the velocity-field curve of $Si_{0.8}Ge_{0.2}$. For Fig. 2(a) we have chosen the alloy potential as 0.2 eV (i.e., half of the band-gap difference between Si and Ge). From Fig. 2(b) it can be seen that it is important to quantify the alloy potential. The out-of-plane transport for holes is also improved, but to a lesser extent than for in-plane.

Finally, in Fig. 3 we show the simulation results for electron velocity-field relations for $Si_{0.8}Ge_{0.2}$ and Si, along with experimental points for Si. For the alloy we show both in-plane and out-of-plane transport. The in-plane transport is slightly degraded while the out-of-plane transport is improved. Two aspects contribute to this improvement in the

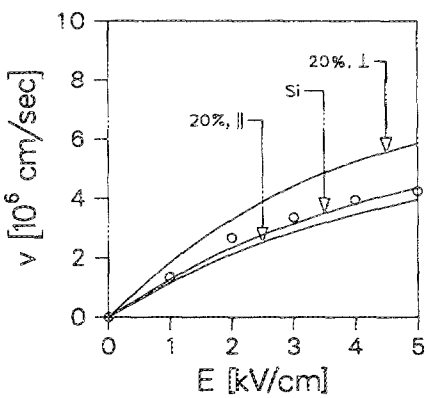

FIG. 3. Electron velocity-field relations for Si, in plane (along [100]) $Si_{0.8}Ge_{0.2}$//(001)Si (20% ∥) and out of plane (along [001]) $Si_{0.8}Ge_{0.2}$//(001)Si (20% ⊥). Experimental points are shown (circles) for Si.

perpendicular transport. First, the band-edge splitting allows a high fraction of carriers to be in the lowered in-plane x valleys which have a lower transverse (in the field direction) effective mass. Second, the intervalley scattering is suppressed due to the splitting of the in-plane and out-of-plane X valleys. On the other hand, for in-plane electron transport, the longitudinal mass of the in-plane valleys dominates the transport and since the mass is higher than the conduction-band-edge density-of-states effective mass in Si, the transport deteriorates somewhat.

In summary, we have presented calculations for basic electron and hole transport in Si-Ge alloys. Both in-plane and out-of-plane hole transport in $Si_{1-x}Ge_x$//Si (001) show increasing mobility with Ge mole fraction x. However, the mobility increase is greater for in-plane than for out-of-plane transport. The out-of-plane electron transport also shows considerable improvements over that of bulk Si. Although several reports of improved device performance in this system have been made, experimental details in transport are still not clear. In particular, the alloy potential used by us is not well characterized experimentally. A need of further experimental investigations of the nature of alloy scattering in this system is indicated. It is hoped that our results will provide motivation for such experimental studies.

This work was supported by the U. S. Army Research Office (grant DAAL03-87-K-0007). The authors also gratefully acknowledge support from the San Diego Supercomputer Center and support from an IBM grant.

[1]T. E. Zipperian, L. R. Dawson, T. J. Drummond, J. E. Shirber, and J. J. Fritz, Appl. Phys. Lett. **53**, 975 (1988).
[2]C. P. Lee, W. T. Wang, G. J. Sullivan, N. H. Sheng, and D. L. Miller, IEEE Electron Device Lett. **EDL-8**, 85 (1987).
[3]S. Tiwari and W. Wang, IEEE Electron Device Lett. **EDL-5**, 333 (1984).
[4]Y. J. Chan, D. Pavlidis, M. Razeghi, M. Jaffe, and J. Singh, 15th International GaAs and Related Compounds Conference, Atlanta, 1988 (to be published).
[5]S. C. Hong, G. Kothiyal, N. Debbar, P. Bhattacharya, and J. Singh, Phys. Rev. B **37**, 878 (1988).
[6]S. Smith and A. D. Welbourn, in *Proceedings of the 1987 Bipolar Circuits and Technology Meeting*, Sept. 21–22, 1987, edited by J. Jopke, (IEEE Electron Device Society, Minneapolis, 1987), p. 57.
[7]T. Taksumi, H. Hirayama, and A. Aiziaki, Appl. Phys. Lett. **52**, 895 (1988).
[8]H. Temkin, Z. C. Bean, A. Antreasyan, and R. Leibengulth, Appl. Phys. Lett. **52**, 1089 (1988).
[9]G. L. Patton, S. S. Iyer, S. L. Delage, S. Tiwari, and J. M. C. Stork, IEEE Electron Device Lett. **9**, 165 (1988).
[10]T. Won and H. Morkoc, IEEE Trans. Electron Device **10**, 33 (1989).
[11]J. D. Wiley, Phys. Rev. B **4**, 2485 (1971).
[12]M. Costato and L. Reggiani, Phys. Status Solidi B **58**, 461 (1973).
[13]K. Brennen and K. Hess, Phys. Rev. B **29**, 5581 (1984).
[14]J. Hinckley and J. Singh, Appl. Phys. Lett. **53**, 785 (1988).
[15]F. Madarasz and F. Szmulowicz, Phys. Rev. B **24**, 4611 (1981).
[16]J. W. Harrison and J. R. Hauser, Phys. Rev. B **13**, 5347 (1976).
[17]E. J. Ryder, Phys. Rev. **90**, 766 (1953).
[18]A. Alberigi-Quaranta, M. Martini, G. Ottaviani, G. Redaelli, and G. Zanarini, Solid State Commun. **11**, 685 (1968).