Hole effective mass in strained $Si_{1-x}C_x$ alloys

C. Y. Lin[a)]
Department of Physics, National Chung Hsing University, Taichung, Taiwan, Republic of China

S. T. Chang
Department of Electronic Engineering, Chung Yuan Christian University, Chungli, Taiwan, Republic of China

C. W. Liu
Department of Electrical Engineering and Graduatė Institute of Electronic Engineering, National Taiwan University, Taipei, Taiwan, Republic of China

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The directional, density-of-states, and carrier-concentration effective masses of light, heavy, and split-off holes have been calculated for strained $Si_{1-x}C_x$ alloys on Si (001) substrate. The results for the directional effective mass show that the effect of strain makes the constant energy surface of light holes near the band edge more symmetric than that in pure silicon. The effect of strain on the heavy and split-off hole bands is rather regular; up to 7% of carbon concentration the strain effect monotonically reduces the density-of-states effective mass for the two bands at energy values within energy interval of 0.4 eV below the valence band edge. This reduction is obtained for the carrier-concentration effective mass at temperatures from 0 to 600 K. The strain effect on the light hole band is less trivial; at nonzero carbon concentrations the strain effect influences the density-of-states and the carrier-concentration effective mass in a similar way as it does to the heavy and split-off bands but irregular behavior shows up in the energy interval of 0.02 eV below the valence band edge and at the temperature range from 0 to 140 K. At 7% of carbon doping the total density-of-states effective mass for holes at 77 and 300 K are almost the same, namely, the values are 0.39 and 0.40 in units of free electron mass, respectively. © *2004 American Institute of Physics*. [DOI: 10.1063/1.1796516]

I. INTRODUCTION

The directional, density-of-states (DOS), and carrier-concentration (CC) effective masses of carriers, are important and fundamental parameters of the transport properties of semiconductors.[1–3] The directional effective mass, which is related directly to the curvature of the constant energy surface, provides information on anisotropy of mobility. The DOS effective mass m_{DOS} is obtained from the density of states and is energy dependent. The CC effective mass m_{CC} is obtained from the carrier concentration and depends both on temperature and Fermi level. The dependence of m_{CC} on Fermi level becomes insignificant for nondegenerate semiconductors. The knowledge of these parameters is essential to the modeling of transport and optical phenomena in semiconductors. In applications of group IV alloys, the effect of strain producing favorable transport and optical properties, has been observed in strained $Si_{1-x}Ge_x$ layer pseudomorphically grown on (001) Si substrate.[4–7] Recently, the optical and electronic properties of strained $Si_{1-x}C_x$ and $Si_{1-y}Ge_xC_y$ on Si substrates have attracted much interest.[8–14] Compared to strained $Si_{1-x}Ge_x$ alloys on Si substrates, since the lattice constant of $Si_{1-x}C_x$ alloy is smaller than that of Si, it is the tensile strain that acts on the $Si_{1-x}C_x$ alloy rather than compressive strain. Also, since the atomic size of carbon is only about half of that of Si, relatively smaller amount of carbon doping creates considerable effect of strain in the strained $Si_{1-x}C_x$ alloy grown on Si substrate. The energy band structure of strained $Si_{1-x}C_x$ alloys on Si(001) substrates has been calculated based on a 20×20 Hamiltonian matrix constructed from the linear combination of atomic orbital (LCAO) approximation with spin-orbit interaction, strain effect, and lattice disorder effect taken into account.[15] The results show that the strain effect removes the degeneracy at Γ point leaving the valence band edge monopolized by the light hole band. In this work all directional effective mass, m_{DOS}, and m_{CC} of strained $Si_{1-x}C_x$ alloys are calculated based on the LCAO energy band structure proposed in Ref. 15. The m_{CC} is evaluated only for the nondegenerate case.

II. EVALUATION OF THE DIRECTIONAL EFFECTIVE MASS

By using the LCAO energy band structure,[15] the directional effective masses are calculated from the energy curvature in the standard fashion by

$$\frac{1}{m_i}=\frac{1}{\hbar^2}\left(\frac{\partial^2 E}{\partial k_i^2}\right), \tag{1}$$

where the index i indicates the direction of interest. Using Eq. (1), the angular dependence of the directional effective masses are obtained in Figs. 1(a)–1(d) for bulk Si and in Figs. 1(e) and 1(f) for strained $Si_{0.99}C_{0.01}$ on Si. Figures 1(a) and 1(b) show the angular dependence of the Si light hole directional effective masses for two constant energy surfaces

a)Author to whom correspondence should be addressed; electronic mail: cylin@nchu.edu.tw

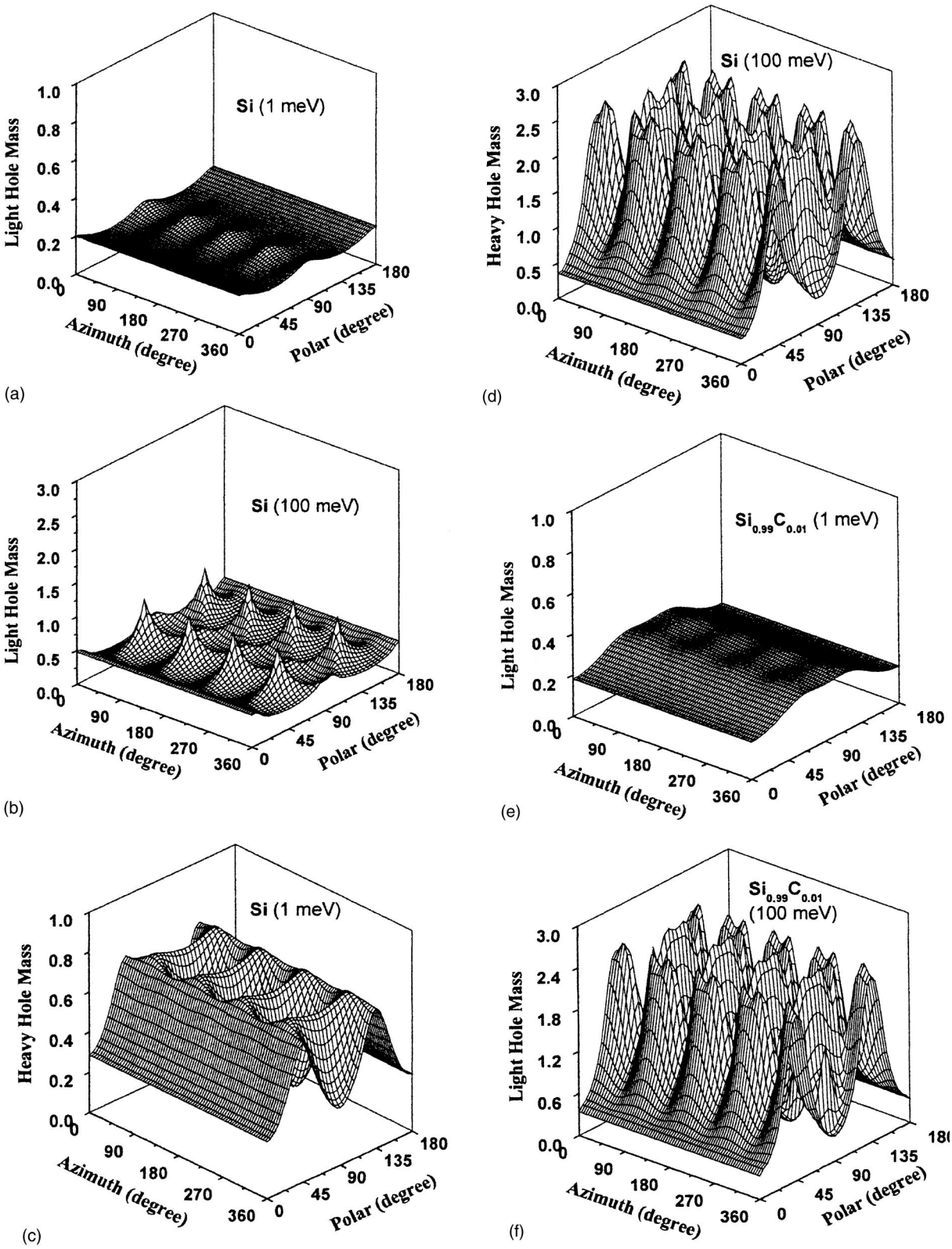

FIG. 1. Angular dependence of the directional effective masses. The light hole band directional effective masses of Si are at the equienergy surfaces of (a) 1 meV and (b) 100 meV. The heavy hole band directional effective masses of Si are at the equienergy surfaces of (c) 1 meV and (d) 100 meV. The light hole band directional effective masses of strained $Si_{0.99}C_{0.01}$ grown on (001) crystallographic plane of Si are at the equi-energy surfaces of (e) 1 meV and (f) 100 meV.

at 1 and 100 meV, respectively, and Figs. 1(c) and 1(d) show Si heavy hole directional effective masses for constant energy surface at 1 and 100 meV, respectively, indicating that the constant energy surface for both light and heavy holes are more warped as the energy increases. For strained $Si_{0.99}C_{0.01}$, there is a different angular dependence of the directional masses. Very close to the valence band edge, as shown in Fig. 1(e), the directional masses are nearly constant along the

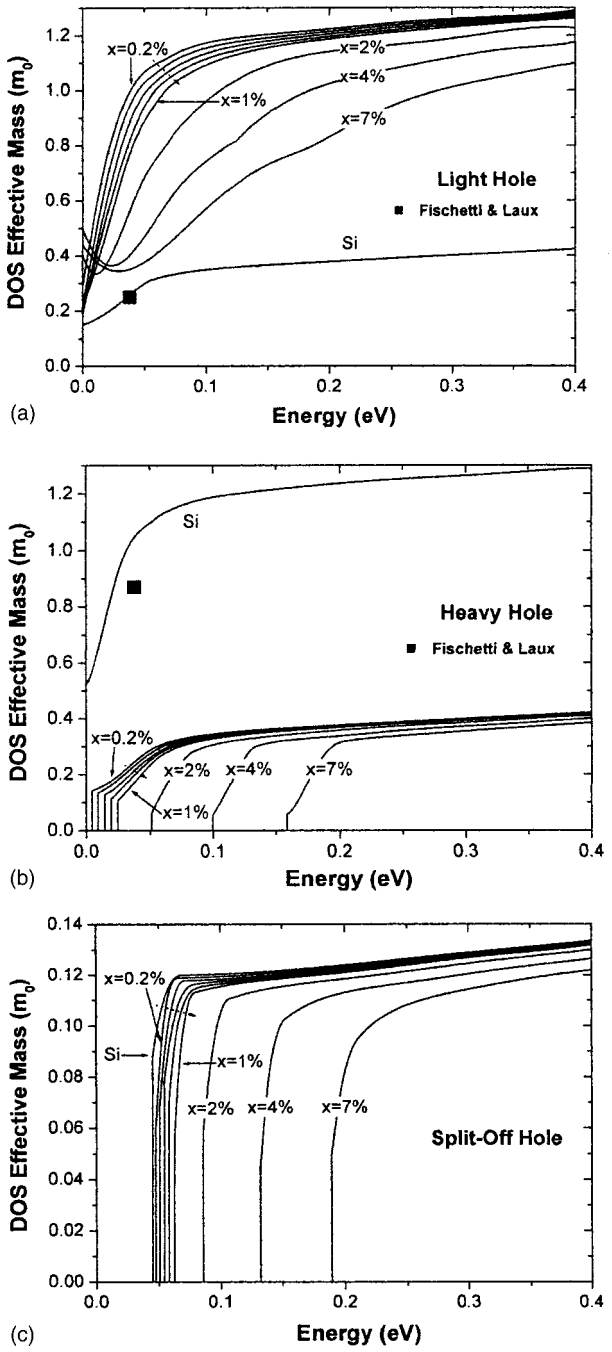

FIG. 2. The DOS effective mass m_{DOS} (in units of the free electron mass) of strained $Si_{1-x}C_x$. The unlabeled curves between the $x=0.2\%$ and $x=1\%$ curves correspond consecutively to $x=0.4\%$, 0.6%, and 0.8%, respectively. Results of Fischetti and Laux (see Ref. 16) (using nonlocal empirical pseudopotential method) for light and heavy hole bands of bulk Si at room temperature thermal energy $(3/2)k_BT$ (where $T=300$ K) are shown for comparison. (a) For the light hole band. (b) For the heavy hole band. (c) For the split-off hole band.

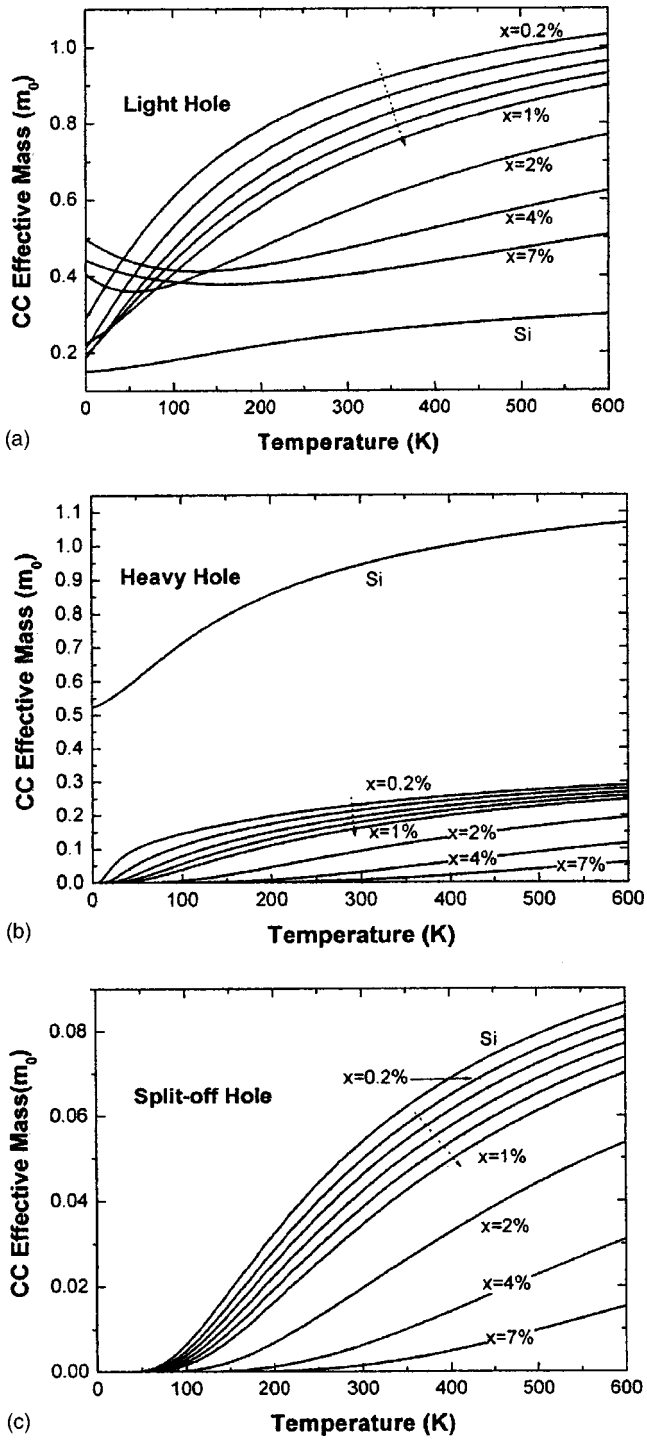

FIG. 3. The CC effective mass m_{CC} (in units of the free electron mass) of strained $Si_{1-x}C_x$. The unlabeled curves between the $x=0.2\%$ and $x=1\%$ curves correspond consecutively to $x=0.4\%$, 0.6%, and 0.8%, respectively. (a) For the light hole band. (b) For the heavy hole band. (c) For the split-off hole band.

azimuthal angle, i.e., on the plane normal to growth direction and show a small change along the polar angle. Compared to Figs. 1(a) and 1(c) we see that energy surface near the valence band edge for strained $Si_{1-x}C_x$ alloy is more symmetrical (in fact it is an ellipsoid) than that for pure Si. The angular dependence of the directional masses of the strained $Si_{0.99}C_{0.01}$ shown in Fig. 1(f) becomes similar to that of heavy hole of bulk Si at higher energy as shown in Fig. 1(d). These changes of the angular dependence of the directional effective masses under strain imply the possible anisotropy of the mobility. Expressing the effective mass in units of free electron mass m_0, our result of the directional effective mass of bulk Si averaged over all the directions for heavy hole is 0.518 at 1 meV and 1.15 at 100 meV.

III. EVALUATION OF THE DENSITY-OF-STATES EFFECTIVE MASS m_{DOS}

Following a similar approach given by Refs. 1 and 2, the $m_{DOS}(E)$ in units of m_0, as a function of energy E is calculated by

$$m_{DOS}(E) = \frac{\hbar^2}{2}\left(\frac{1}{2\pi\sqrt{E}}\frac{dV}{dE}\right)^{2/3}, \tag{2}$$

where $V(E)$ is the volume of a constant energy shell that is calculated by the integral

$$V(E) = \frac{1}{3}\int_0^{\pi} \sin\theta d\theta \int_0^{2\pi} d\phi k^3(E,\theta,\phi), \tag{3}$$

where k, θ, and ϕ denote the spherical polar coordinates. The function $k(E,\theta,\phi)$, which is the k-space radial size of constant E surface along the direction of (θ,ϕ), is solved from the corresponding LCAO Hamiltonian matrix[15] of the strained $Si_{1-x}C_x$ alloys.

In terms of energy the DOS effective masses for the light, heavy, and split-off hole bands are shown in Fig. 2 for various values of carbon contents x. For light holes, as shown in Fig. 2(a), the DOS masses decrease monotonically as the strain increases for cases of nonvanishing strains. However, there is a leap of the DOS mass values at the introduction of strain to the bulk Si. This is due to the fact that the valence band edge is assigned to be taken by the light hole band, in the same way as the degeneracy at the band edge in bulk Si is removed by the strain.[15] Therefore, for each given energy the light hole band in strained $Si_{1-x}C_x$ corresponds to the largest constant energy surface in k space, similarly as the heavy hole band does in the bulk Si. The largest-in-size constant energy surface in k space for the light hole band when strain effect is taken into account consequentially makes its DOS effective mass larger than that of the heavy hole band. Similar to the situation found in light hole band of strained $Si_{1-x}Ge_x$ in Ref. 2 the crossing dips are observed at lower energies for higher carbon concentrations $2\% \leqslant x \leqslant 7\%$. As shown in Figs. 2(b) and 2(c), the heavy and the split-off hole DOS masses decrease monotonically as the strain increases. Our results of DOS effective mass for light and heavy hole bands of bulk Si, based on the LCAO approximation, at room temperature thermal energy $(3/2)k_BT$ (where k_B is Boltzmann constant and $T=300$ K), are in good agreement with those calculated from the nonlocal empirical pseudopotential method.[16]

IV. EVALUATION OF THE CARRIER-CONCENTRATION EFFECTIVE MASS M_{CC}

Following the expression derived in Ref. 1 the carrier-concentration effective mass $m_{CC}(\mu,T)$, being a function of Fermi level μ and temperature T, can be calculated in terms of DOS effective mass from formula

$$m_{cc}^{3/2}(\mu,T) = \frac{\beta^{3/2}}{F_{1/2}(\beta\mu)}\int_0^{\infty} \frac{m_{DOS}^{3/2}(E)E^{1/2}}{1+\exp[\beta(E-\mu)]}dE, \tag{4}$$

where $F_{1/2}$ is a Fermi integral[17] F_n of order $n=1/2$ and $\beta = (k_BT)^{-1}$. The above expression can be simplified if the Fermi level is sufficiently negative, namely, in the case of $\mu < -3k_BT$. In this case Eq. (4) reduces to

$$m_{cc}^{3/2}(T) = \frac{2\beta^{3/2}}{\sqrt{\pi}}\int_0^{\infty} m_{DOS}^{3/2}(E)E^{1/2}\exp(-\beta E)dE. \tag{5}$$

We calculate the m_{CC} only for the nondegenerate case.

Results of the carrier-concentration effective mass, as a function of temperature for various carbon contents, are shown in Fig. 3 for the light hole (LH), heavy hole (HH), and split-off hole (SH) bands. The fact that the DOS effective mass of light hole band is larger than that of heavy hole band when strain effect is taken into account in turn results in a larger CC effective mass for light hole band. In the temperature range from 0 to 600 K, the CC effective masses for HH and SH bands decrease monotonically as the carbon fraction increases. The CC effective masses for LH band behave the same way except in the temperature range of 0–140 K. The result of total density-of-states effective mass for holes m_{dh}, which is defined as

$$m_{dh} = (m_{cc,LH}^{3/2} + m_{cc,HH}^{3/2} + m_{cc,SH}^{3/2})\exp(-\Delta_{SO}/k_BT)^{2/3}, \tag{6}$$

where Δ_{so} is the spin-orbit splitting, is shown in Fig. 4. For carbon content less than 1% m_{dh} increases monotonically as temperature increases and decreases monotonically as the strain effect increases. For carbon content $x \geqslant 1\%$, m_{dh} behaves in a more complex fashion in low temperature range below 140 K, due to stronger strain effects.

m_{dh} as a function of carbon composition ($x \leqslant 0.07$), for two common operating temperatures in semiconductor devices, is shown in Fig. 5. For pure Si ($x=0$) at 300 K our result of $1.04m_0$ matches well with the well-known value of $1.1m_0$. m_{dh} for both temperatures 300 and 77 K tend to saturate as the strain effect gets stronger and the values are approaching to each other, when the carbon content increases. m_{dh} at the two temperatures are then almost the same at 7% of carbon doping; they are $0.40m_0$ at 300 K and $0.39m_0$ at 77 K.

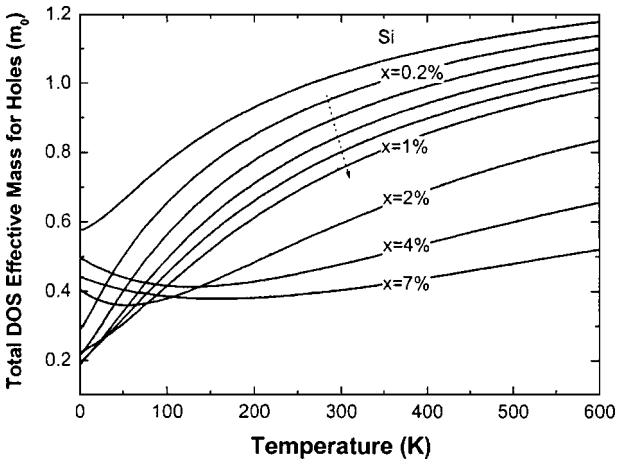

FIG. 4. The total density-of-states effective mass for holes m_{dh} (in units of the free electron mass) of strained $Si_{1-x}C_x$ as a function of temperature. The unlabeled curves between the $x=0.2\%$ and $x=1\%$ curves correspond consecutively to $x=0.4\%$, 0.6%, and 0.8%, respectively.

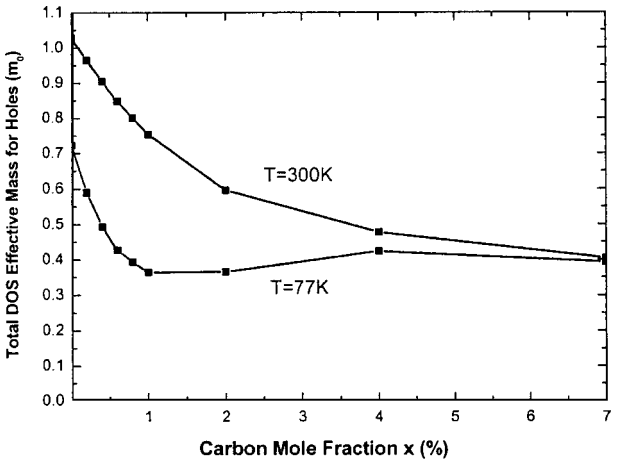

FIG. 5. The total density-of-states effective mass for holes m_{dh} of strained $Si_{1-x}C_x$ as a function of C mole fraction for 77 and 300 K.

V. SUMMARY

In this work we report calculated results of directional, DOS, and CC effective masses of strained $Si_{1-x}C_x$ alloys, with up to 7% of carbon concentration, with energy ranging from the valence band edge down to the energy of 0.4 eV below this edge. The effect of strain removed the degeneracy at Γ point leaving the valence band edge monopolized only by an ellipsoidal light hole band. The DOS and CC effective masses for heavy hole and split-off hole bands decrease monotonically as the strain effect increases. The strain effect on the light hole band is more complex. For lower carbon concentrations, $0.2\% \leqslant x \leqslant 1\%$, the DOS effective mass as a function of energy decreases as the strain increases, but crossing dips are observed near the valence band edge at higher carbon concentrations, $2\% \leqslant x \leqslant 7\%$. The CC effective mass of light hole band, as a function of temperature, behaves similarly; for $0.2\% \leqslant x \leqslant 1\%$ m_{CC} decreases monotonically as the strain effect increases, but crossing dips are also observed at low temperatures for $2\% \leqslant x \leqslant 7\%$. For temperature at 300 and 77 K, the value of m_{dh}, as a function of carbon concentration x, tends to saturate to the same value, as the strain effect increases.

ACKNOWLEDGMENTS

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