# Energy and temperature dependence of electron effective masses in silicon

Nicolas Cavassilas, Jean-Luc Autran, Frédéric Aniel, and Guy Fishman

Citation: Journal of Applied Physics **92**, 1431 (2002); doi: 10.1063/1.1490620
View online: http://dx.doi.org/10.1063/1.1490620
View Table of Contents: http://scitation.aip.org/content/aip/journal/jap/92/3?ver=pdfcov
Published by the AIP Publishing

# Energy and temperature dependence of electron effective masses in silicon

Nicolas Cavassilas[a] and Jean-Luc Autran
*Laboratoire Matériaux et Microélectronique de Provence (L2MP, UMR CNRS 6137), Bâtiment IRPHE, 49 Rue Joliot–Curie, Boîte Postale 146, F-13384 Marseille, Cedex 13, France*

Frédéric Aniel and Guy Fishman
*Institut d'Electronique Fondamentale (IEF, UMR CNRS 8622), Université Paris XI, F-91405 Orsay Cedex, France*

(Received 26 February 2002; accepted for publication 8 May 2002)

A $\mathbf{k}\cdot\mathbf{p}$ model is used to theoretically investigate the energy and lattice temperature dependence of both transverse and longitudinal ''curvature'' electron effective masses in silicon. The temperature dependence of the carrier concentration conduction effective masses in the range of 10–550 K is also examined. Our results highlight the energy dependence of the longitudinal effective mass, usually considered to be equal to the band-edge effective mass, which varies from 0.917 to $1.6m_0$ when the carrier energy ranges from the bottom of the conduction band up to 1.5 eV. This energy dependence should have a significant impact on electronic transport simulations using drift–diffusion, hydrodynamic, or Monte Carlo methods, particularly for hot-carrier phenomena in microelectronic devices. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1490620]

## I. INTRODUCTION

Much effort has been made to introduce the nonparabolic nature of band structures into semiconductor device simulators.[1,2] In order to account for this nonparabolic band structure, a full-band model should be rigorously considered, but this remains marginally tractable from a computational point of view. An alternative approach consists of using two distinct sets of effective masses.[2] The first one is related to the ''curvature'' band masses obtained from the derivative of the dispersion relationship in various directions away from the valley minima. These masses are called the ''curvature electron effective masses'' ($m^{\mathrm{cur}}$). They are energy dependent, and are equal to the well-known band-edge effective masses $m^*$ at the valley minima. The second one concerns the carrier concentration effective masses ($m^{\mathrm{cc}}$) which correspond to average values integrated over thermal equilibrium carrier distributions. These masses are temperature dependent. The energy and temperature dependences of these two sets of masses arises from the nonparabolic nature of the band, and they may significantly impact simulation results. For example, the energy dependence of $m^{\mathrm{cur}}$ may become important in considering hot carrier phenomena in Monte Carlo simulations (the ballistic and scattering rates) of semiconductor devices. On the other hand, the temperature dependence of $m^{\mathrm{cc}}$ should be taken into account, for example, in the calculation of the intrinsic carrier density versus temperature.

A full-band computation of the carrier dispersion relation in the semiconductor is required for complete calculation of these effective masses, and it is generally obtained through a $\mathbf{k}\cdot\mathbf{p}$ approach. Compared to empirical pseudopotential or tight-binding methods, $\mathbf{k}\cdot\mathbf{p}$ theory has been found to be a very efficient and convenient approach[3,4] by which to calculate such band structures. But, until recently, $\mathbf{k}\cdot\mathbf{p}$ theory could not correctly treat the conduction band in an indirect band gap semiconductor such as silicon and, consequently, complete calculations of $m^{\mathrm{cur}}$ and $m^{\mathrm{cc}}$ reported in the literature only concerned holes.[2] Recently, a $sps^*$ $\mathbf{k}\cdot\mathbf{p}$ model was proposed as an efficient way to calculate the complete band structure (conduction *and* valence bands) over the entire Brillouin zone in direct *and* indirect semiconductors for energies of interest in hot-carrier transport phenomena.[4] In the present work, we propose a complete calculation of $m^{\mathrm{cur}}$ and $m^{\mathrm{cc}}$ for the conduction band of silicon using this approach.

## II. BAND-STRUCTURE CALCULATION

First, we present calculation of the complete band structure of Si in a lattice temperature range of 10–550 K. The temperature-dependent quantities considered in the $\mathbf{k}\cdot\mathbf{p}$ model are the lattice constant[5] and the two band-band transitions, $\Gamma_6^- - \Gamma_8^+$ and $\Gamma_7^- - \Gamma_8^+$, i.e., the direct band gaps.[4] The lattice temperature dependence of these energies was determined via an iterative process until the indirect band gap $E_G$ given by the $\mathbf{k}\cdot\mathbf{p}$ algorithm fit experimental data[6,7] as illustrated in Fig. 1. This ''inverse model'' approach allowed us to quantify the impact of the lattice temperature on the shape of the $\Delta$ valley (i.e., the minimum of the conduction band) which is conventionally assumed to be an ellipsoid with longitudinal and transverse directions. For each direction, the following dispersion equation is assumed:

$$k_{l,t}^2 = \frac{2m_0}{\hbar^2} f_{l,t}(E), \tag{1}$$

where $m_0$ is the free electron mass, $k_{l,t}$ is the wave vector in the transverse ($t$) or in the longitudinal ($l$) direction, $E$ is the energy, and $f_{l,t}$ is a function of the energy. The curvature effective mass is defined as the derivative of the $E-k^2$ curve,

[a]Electronic mail: cavassil@newsup.univ-mrs.fr

 

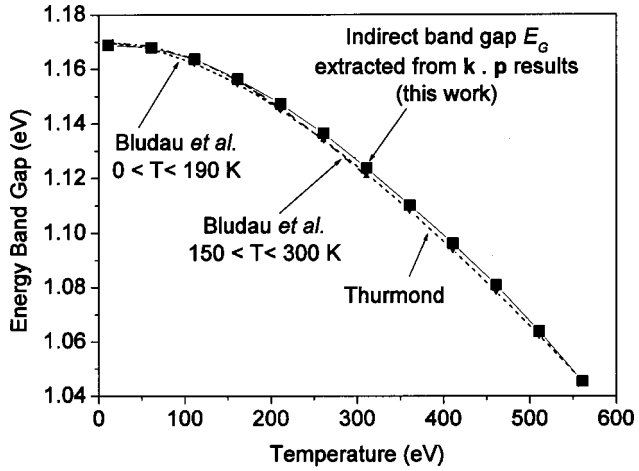


FIG. 1. Indirect energy band gap of Si vs lattice temperature extracted from the $\mathbf{k}\cdot\mathbf{p}$ calculation and compared to experimental results given by Bludau *et al.* (see Ref. 6) (two fits, respectively, for 0–190 and 150–300 K) and by Thurmond (see Ref. 7) (200–1200 K).

$$\frac{m_{l,t}^{\mathrm{cur}}(E)}{m_0}=\frac{df_{l,t}(E)}{dE}. \tag{2}$$

The transverse and longitudinal band edge effective masses $m^*$ calculated are shown in Fig. 2 as a function of the lattice temperature. The energy dependence of the corresponding transverse and longitudinal curvature effective masses $m_{l,t}^{\mathrm{cur}}(E)$ is given in Fig. 3 for different values of the lattice temperature. The first unexpected result is the weak temperature dependence of these masses. Consequently, the temperature dependence of the band structure can be reasonably approximated by considering only the variation of the energy band gap with the temperature. Another important result concerns $m_l^{\mathrm{cur}}$ which is often considered energy independent (i.e., the $\Delta$ valley is treated as parabolic in the longitudinal direction).[1,8,9] This hypothesis is in disagreement with the calculated Si band structure obtained with pseudopotential,[10] tight-binding,[11] or $\mathbf{k}\cdot\mathbf{p}$ methods[4] (including the present work). In that respect, the results presented in Fig. 3 provide important findings for hot electron transport

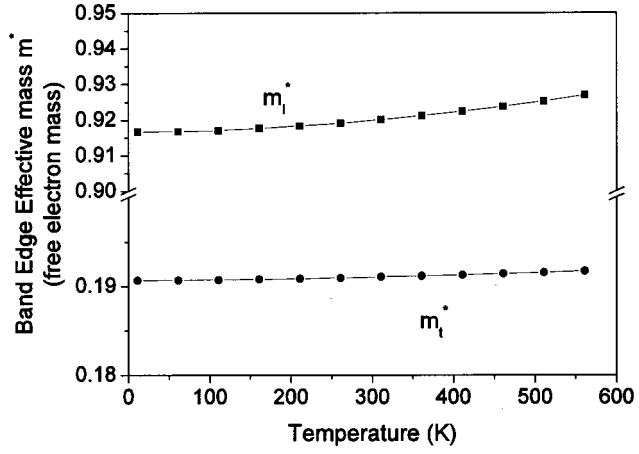


FIG. 2. Band edge effective masses $m_{l,t}^*$ (transverse and longitudinal) of the silicon $\Delta$ valley vs the lattice temperature.

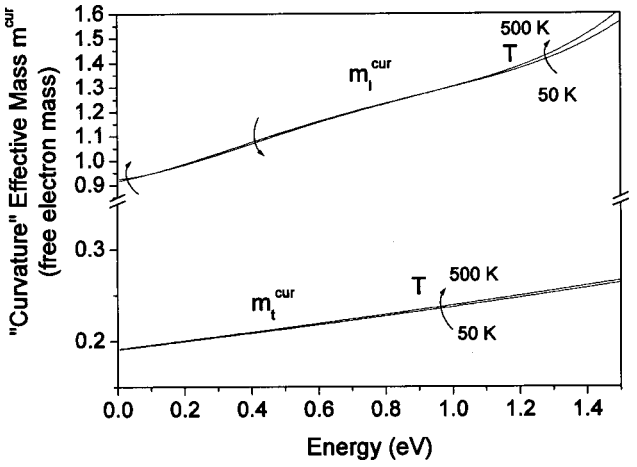


FIG. 3. Curvature effective masses $m_{l,t}^{\mathrm{cur}}$ (transverse and longitudinal) of the silicon $\Delta$ valley vs the energy (from the bottom of the conduction band) calculated for two lattice temperatures ($T=50$ and 500 K).

simulation, particularly for description of electron–phonon interactions in nonfull-band Monte Carlo models, where band-edge effective masses are used by default. In particular, we show in Fig. 3 the theoretical values of $m_l^{\mathrm{cur}}$ and $m_t^{\mathrm{cur}}$ for energies up to 1.5 eV, i.e., high energies compared to the impact ionization threshold in silicon (1.3 eV).[12]

## III. CARRIER CONCENTRATION EFFECTIVE MASSES

The carrier concentration effective masses $m_l^{\mathrm{cc}}$ and $m_t^{\mathrm{cc}}$ can be defined from the curvature band effective masses,[2] i.e.,

$$m_{l,t}^{\mathrm{cc}}(T)^{3/2}=\frac{\int_0^\infty m_{l,t}^{\mathrm{cur}}(E)^{3/2}f(E,E_F)E^{1/2}dE}{\int_0^\infty f(E,E_F)E^{1/2}dE}, \tag{3}$$

where $f(E,E_F)$ is the Fermi–Dirac distribution function and $E_F$ is the Fermi level, with the carrier temperature equal to the lattice temperature. $m_l^{\mathrm{cc}}$ and $m_t^{\mathrm{cc}}$ are shown in Fig. 4 as a function of the lattice temperature in the range of 10–550 K and for different values of the Fermi level. In order to compare these results with Vankammel *et al.*'s analytical fit[13] (based on Barber's data[1]), the spherical carrier concentration effective mass, which corresponds to the geometric mean of $m_l^{\mathrm{cc}}$ and $m_t^{\mathrm{cc}}$ over the three axes, was also computed, i.e.,

$$m_{\mathrm{spherical}}^{\mathrm{cc}}=K^{2/3}(m_l^{\mathrm{cc}}m_t^{\mathrm{cc}^2})^{1/3}, \tag{4}$$

where $K=6$ is the number of $\Delta$ valley minima in silicon.

As seen from Fig. 4, Barber's mass shows a more pronounced temperature dependence compared to our calculations. It might be explained by the fact that Barber's data are derived from cyclotron resonance measurements at low temperatures[8] and Faraday effect measurements at higher temperatures.[14] As reported by Green,[9] a closer examination of these Faraday experiments[14] shows that the relatively large effective mass increases with the temperature might result from the temperature dependence of the Hall factor for electrons, which was assumed to be constant in Ukhanov and Mal'tsev's work.[14] More reliable measurements of the temperature dependence of the transverse mass performed by Ousset *et al.*[15] give values that are in very good agreement

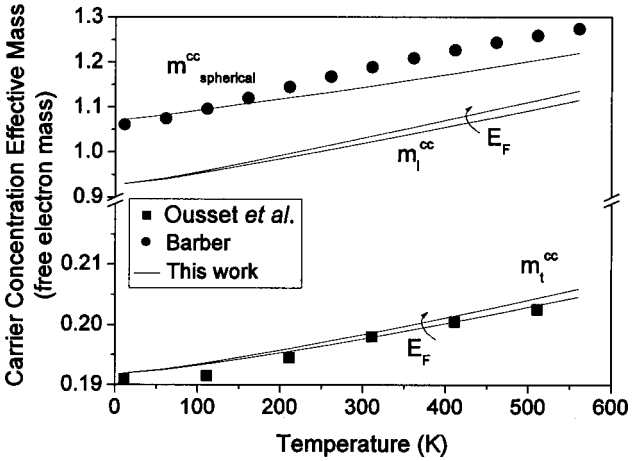


FIG. 4. Carrier concentration effective masses $m_{l,t}^{cc}$ (transverse and longitudinal) of the silicon Δ valley vs the temperature calculated for two different positions of the Fermi level with respect to the bottom of the conduction band: $E_F=-0.2$ and 0.0 eV. The spherical $m^{cc}$ obtained from Eq. (4) and for $E_F=-0.2$ eV (the nondegenerate limit) is compared to Barber's results reported in Ref. 13. The transverse mass is also compared to the experimental result given by Ousset *et al.* (see Ref. 15).

with our computation (see Fig. 4). With regard to the temperature dependence of the longitudinal mass, to the best of our knowledge, there are no experimental data available for comparison. Finally, Fig. 4 shows that the temperature dependence of $m^{cc}$ increases when $E_F$ is pushed closer to the conduction band. At the same time, one notices that $m^{cc}$ becomes independent of the Fermi level if $E_F$ is more than $\sim$0.2 eV from the conduction band, which corresponds to the nondegenerate limit.

## IV. CONCLUSION

We have calculated both the curvature and carrier concentration effective masses in the conduction band of silicon. These masses were found to be, respectively, energy and temperature dependent, due to the nonparabolic nature of the conduction band which was accurately determined from a $\mathbf{k}\cdot\mathbf{p}$ approach. A significant finding is the energy dependence of the curvature longitudinal effective mass which was found to vary from 0.917 to $1.6m_0$ from the bottom of the conduction band up to 1.5 eV. Another result concerns the first evaluation of both the longitudinal and transverse carrier concentration masses from rigorous theoretical treatment. These results should be important for the simulation of Si devices using nonfull-band models.

[1] H. D. Barber, Solid-State Electron. **10**, 1039 (1967).
[2] F. L. Madarasz, J. E. Lang, and P. M. Hemeger, J. Appl. Phys. **52**, 4646 (1981).
[3] Z. Ikonic, R. W. Kelsall, and P. Harrison, Proceedings of the 25th International Conference on the Physics of Semiconductors, 2001, 479.
[4] N. Cavassilas, F. Aniel, K. Boujdaria, and G. Fishman, Phys. Rev. B **64**, 115207 (2001).
[5] *Semiconductors: Intrinsic Properties of Group IV Elements and III–V, II–VI and I–VII Compounds*, edited by O. Madelung, Landolt-Börnstein, New Series, Group III, Vol. 22, Part a (Springer, Berlin, 1987).
[6] W. Bludau, A. Onton, and W. Heinke, J. Appl. Phys. **45**, 1846 (1974).
[7] C. D. Thurmond, J. Electrochem. Soc. **122**, 1133 (1975).
[8] R. A. Stradling and V. V. Zhukov, Proc. Phys. Soc. London **87**, 263 (1966).
[9] M. A. Green, J. Appl. Phys. **67**, 2944 (1989).
[10] M. L. Cohen and J. R. Chelikowsky, *Electronic Structure and Optical Properties of Semiconductors*, Springer Series in Solid State Sciences, edited by M. Cardona (1989).
[11] J. M. Jancu, R. Scholz, F. Beltram, and F. Bassani, Phys. Rev. B **57**, 6493 (1998).
[12] M. V. Fischetti, N. Sano, S. E. Laux, K. Natori, IEEE Trans. Semicond. Technol. Modeling Simul., URL: http://www.ieee.org/journal/tcad/accepted/fischetti-feb97/.
[13] R. Vankemmel, W. Schoenmaker, and K. De Meyer, Solid-State Electron. **36**, 1379 (1993).
[14] Yu. I. Ukhanov and Yu. V. Mal'tsev, Sov. Phys. Solid State **5**, 2144 (1964).
[15] J. C. Ousset, J. Leotin, S. Askenazy, M. S. Skolnick, and R. A. Stradling, J. Phys. C **C9**, 2803 (1976).