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Deformation-potential-theory calculation of the acoustic-phonon-limited conductivity and Hall mobilities for p-type silicon

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Acoustic-phonon-limited conductivity and Hall mobilities of p-type silicon are calculated for the first time within the framework of the deformation potential theory of Tiersten. We solve the Boltzmann equation for the distribution function using hole–acoustic-phonon transition rates which are functions of hole energies and incident and scattered hole wave vectors. We employ no band-shape approximations and use deformation-potential parameters from independent experiments. The calculated mobilities are in excellent agreement with experiments without any empirical adjustment of input parameters.

Phonon-limited-transport calculations for p-type nonpolar semiconductors had attained a high degree of sophistication with rigorous implementations of the deformation-potential theory for germanium by Tiersten[1] and Lawaetz.[2] This approach has hence not been pursued in favor of less exact models where the fundamental input parameters, the deformation potentials, became regarded as empirically adjustable in order to fit the data.[3–12] Moreover, no attempts have been made since to go beyond the relaxation time approximation in solving the Boltzmann equation. In this work we reinitiate calculations within the more exact model for silicon without any band shape approximations, using the hole–acoustic-phonon transition rates from the deformation-potential theory of Tiersten,[1] no relaxation time approximation, and no adjustable parameters.

The conductivity and Hall mobilities are calculated from the low-field expansion of the average thermal velocity[2]

$$\langle\vec{V}\rangle=\frac{\sum_{\vec{k}}\sum_{N}\left(\frac{1}{\hbar}\vec{\nabla}_{\vec{k}}E_N(\vec{k})\right)f_N(\vec{k})}{\sum_{\vec{k}}\sum_{N}f_N(\vec{k})}$$
$$=\mu_c(\vec{F}+\mu_H\vec{F}\times\vec{B}+\cdots)\ , \tag{1}$$

where $f_N(\vec{k})$ is the steady-state distribution function for band N (heavy, light, and spin-orbit valence bands) at wave vector $\vec{k}$ with energy $E_N(\vec{k})$. $\vec{F}$ and $\vec{B}$ are the electric and magnetic fields, respectively. μ_c is the conductivity mobility and μ_H the Hall mobility (their ratio μ_H/μ_c is the so-called r factor). First we must solve the Boltzmann equation

$$\left(\frac{e\vec{F}}{\hbar}\cdot\vec{\nabla}_{\vec{k}}-\frac{e\vec{B}}{\hbar^2}\cdot[\vec{\nabla}_{\vec{k}}E_N(\vec{k})\times\vec{\nabla}_{\vec{k}}]\right)f_N(\vec{k})=\frac{V}{(2\pi)^2}\sum_{M=1}^{3}\int d\vec{k}'\,[f_M(\vec{k}')-f_N(\vec{k})]\,W_{NM}(\vec{k},\vec{k}') \tag{2}$$

for the distribution functions $f_N(\vec{k})$. The scattering term in Eq. (2) contains the transition probability $W_{NM}(\vec{k},\vec{k}')$ for elastic hole scattering from band N at $\vec{k}$ to band M at $\vec{k}'$ with emission or absorption of an acoustic phonon. The transition rates were calculated[13] using the deformation-potential theory of Tiersten[1] with experimentally determined deformation-potential parameters.[14–16] Band dispersions and hole wave functions were obtained from the full 6×6 Kane's $\vec{k}\cdot\vec{p}$ Hamiltonian.[17] The rates were then least-squares fitted[18] to a *double* cubic harmonic expansion in angles $\hat{k}$ and $\hat{k}'$ for each N,M band pair and energies $E_N(\vec{k})=E_M(\vec{k})\equiv E$.

The field expansion of the distribution function takes the form[19]

$$f_N(\vec{k})=f_N^0(\vec{k})[1+\vec{F}\cdot\vec{\Phi}_N(\vec{k})+(\vec{F}\times\vec{B})\cdot\vec{X}_N(\vec{k})+\cdots]\ , \tag{3}$$

where $f_N^0(\vec{k})$ is the Fermi-Dirac distribution function. The coefficients Φ and X are expanded in a single cubic harmonic series for the Γ_{15} representation of O_h (δ_1, δ_3, δ_5, and δ_5' cubic harmonics were used in the expansion of the distribution function).[20] Explicitly,[19]

$$\vec{\Phi}_N(E,\hat{k})=\sum_{\lambda}e\left(\frac{4\pi}{k_BT}\right)^2\vec{K}_\lambda^{\delta}(\hat{k})\,\theta_{N\lambda}^{\delta}(E)\ , \tag{4}$$

$$\vec{X}_N(E,\hat{k})=\sum_{\lambda}\left[\left(\frac{4\pi}{k_BT}\right)^3\frac{4\pi e^2}{\hbar}\right]\vec{K}_\lambda^{\delta}(\hat{k})\,\xi_{N\lambda}^{\delta}(E)\ . \tag{5}$$

Here θ and ξ are energy dependent factors, $\vec{K}$ is a vector with components $K_\lambda^{\delta\nu}(\hat{k})\hat{e}_\nu$, where $K_\lambda^{\delta\nu}(\hat{k})$ is a cubic harmonic transforming like the νth row ($\nu=x,y,z$) of the $\delta=\Gamma_{15}$ irreducible representation of O_h with angular index λ, and $\hat{e}_\nu$ is a unit vector in the νth direction. Inserting the expansions (3)–(5)

in (2) then multiplying both sides of (2) by

$$K_{\lambda'}^{j\mu}(\hat{k})\delta(E_N(\vec{k})-E)\,d\vec{k}\ , \tag{6}$$

and integrating over the whole Brillouin zone, results in two sets of linear inhomogeneous equations for θ and ξ at each energy E. The form of these equations is similar to those derived by Lawaetz,[2] except that our scattering matrix $S_{N\lambda,M\lambda'}(E)$ is symmetric in the combined $N\lambda$ indices.[19] With θ and ξ calculated, the mobilities are obtained as a function of absolute temperature T from Eq. (1).

Our calculational and theoretical approach was tested on germanium using the input parameters of Tiersten[1] and Lawaetz.[2] In the case of μ_c our respective calculations agree to within 7.7%, the small difference here being ascribed to our use of nonparabolic bands versus the parabolic approximation employed in Refs. 1 and 2. Our μ_H is significantly closer to the experimental value than the μ_H calculated by Lawaetz. His 81-K r factor is $r\sim 1.7$, compared to our $r=1.43$, and measured values $r=1.37$,[21] $r=1.27$ (Ref. 22) for high-purity p-type Ge. To be sure, the comparison here is complicated by the fact that optical-phonon scattering becomes significant in germanium for $T>80$ K. Our calculation indicates that the light-hole band contributes overall twice as much as the heavy-hole band to μ_H in spite of its lower thermal hole occupancy. Therefore the nonparabolicity of the light-hole band has to be included accurately in calculation for μ_H. In calculation for μ_c the heavy-hole band contributes four times as much as the light-hole band so that the nonparabolicity of the latter band is not as critical to the final value of conductivity mobility. We surmise that Lawaetz's neglect of the light-hole band's nonparabolicity accounts for the difficulty in his calculation to fit all of the four lowest galvanomagnetic coefficients of Ge with one set of deformation potentials.[2] Lastly, our calculated μ_c agrees to within a couple percent with the relevant data.[23,24]

Figures 1–3 provide the comparison between our calculated results and the most recent data on high-purity p-type silicon in the acoustic-phonon-limited temperature region. Figure 1 shows the r factor and the temperature exponents of both mobilities

$$\mu_{c,H}\sim T^{-\alpha_{c,H}(T)}\ , \tag{7}$$

together with the data of Mitchel and Hemenger[25]

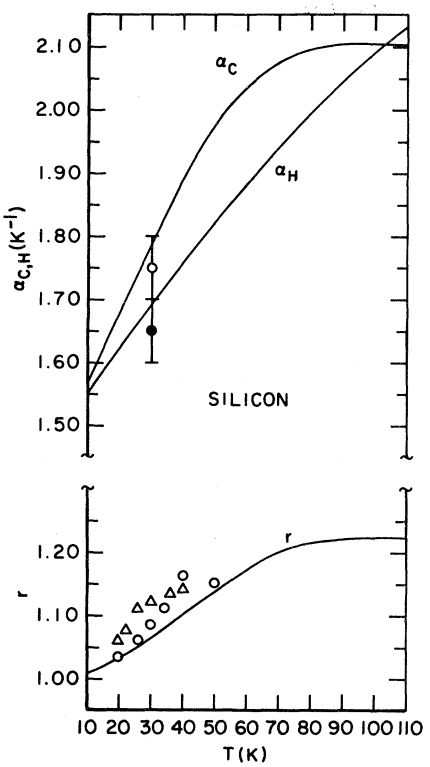

FIG. 1. Calculated and measured temperature exponents for the conductivity mobility α_c and the Hall mobility α_H. Experimental data for α_c (open circle) and α_H (filled circle) from Mitchel and Hemenger (Ref. 25). The r-factor data of Mitchel and Hemenger is from sample 1202-H (triangles, Hall bar acceptors 6.57×10^{11} cm^{-3}, donors 3.96×10^{11} cm^{-3}) and sample 1300-V (circles, Van der Pauw configuration, acceptors 9.14×10^{11} cm^{-3}, donors 3.33×10^{11} cm^{-3}).

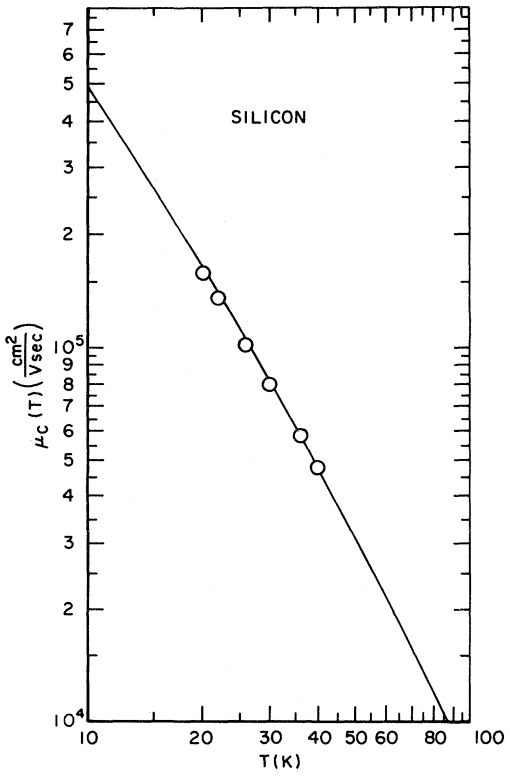

FIG. 2. Calculated conductivity mobility for silicon (solid line) and the experimental data of Mitchel and Hemenger (Ref. 25) for sample 1202-H.

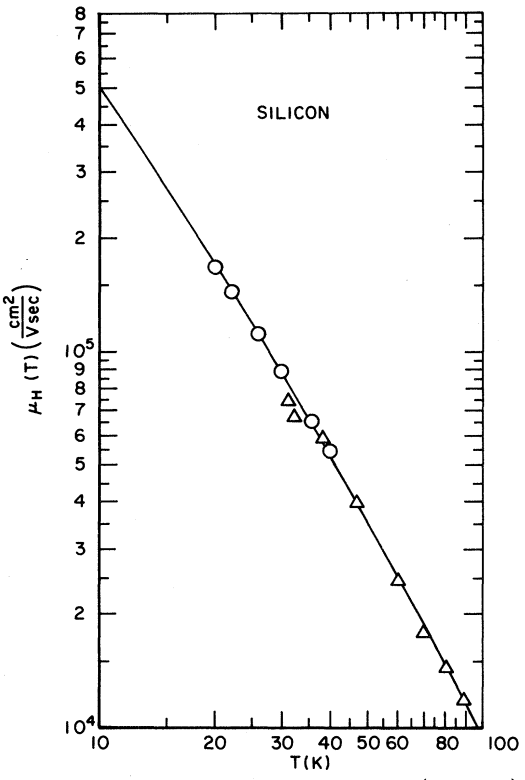

FIG. 3. Calculated Hall mobility for silicon (solid line) and the experimental data of Mitchel and Hemenger (Ref. 25) for sample 1202-H (circles), and the data of Elstner (Ref. 26) (triangles, acceptors 1.0×10^{13} cm^{-3}, donors 6.5×10^{10} cm^{-3}).

(Mitchel *et al.* fitted only one temperature exponent in the 20–40-K range). The calculated and measured exponents are seen to agree quite closely. The *r*-factor data are generally higher than the theory predicts, but the overall agreement is to within 4%, consistent with accuracy of the data.

The μ_c and μ_H curves, Figs. 2 and 3, respectively, are within 2% of the experimental mobilities.[25,26] The agreement is admittedly better than our knowledge of the deformation-potential constants for Si and accuracy of the calculation and theory itself.[2,19,27] For Si we estimate these to produce a $\pm10\%$ limit on the accuracy of the calculation.[2,19,27] For Ge the deformation potentials are not as well known and the set we adopted from Tiersten,[1] for calculational comparison only, appears to be on the high side of the spread of experimental deformation potentials.[14]

In conclusion, we have shown on the examples of Ge and Si that phonon-limited transport in semiconductors can be quantitatively modeled within the deformation-potential theory. With sufficient care taken to incorporate band anisotropies and nonparabolicities in transition rates and band dispersions, together with the use of full Boltzmann equation solutions for the distribution functions, very good agreement with the data can be obtained.

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