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Semiconductor Measurement Technology:

The Dopant Density and Temperature Dependence of Electron Mobility and Resistivity in N-Type Silicon

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LIST OF NOTATIONS*

E electron energy

E_C conduction band edge

E_D donor energy level

E_F Fermi energy

 ${\rm E}_{\rm N}$ $\,$ Binding energy of neutral donors

h Planck's constant (= 6.625×10^{-34})

k Boltzmann's constant (= 1.38×10^{-23})

m free electron mass (= 9.1×10^{-31})

 m_n^* conductivity effective mass

 * Unless stated otherwise, all units are in MKS.

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density of states effective mass m,* longitudinal effective mass m_o* m* transverse effective mass electron density (cm^{-3}) n ^{N}C effective density of conduction band states (cm^{-3}) total donor density (cm⁻³) ND N_{D}^{+} ionized donor density (cm^{-3}) NT net ionized impurity density (cm⁻³) neutral donor density (cm⁻³) NN electronic charge (= 1.6×10^{-19}) P Т absolute temperature free space permittivity (=8.854 \times 10⁻¹²) ε permittivity of silicon (= $11.7 \times \epsilon_{0}$) ε_s donor ionization energy (= $(E_{C} - E_{D})/q eV)$ ε_D lattice scattering mobility (cm²/V·s) μ_{T} ionized impurity scattering mobility (cm²/V·s) μ_T neutral impurity scattering mobility (cm²/V·s) μ_N combined lattice and ionized impurity scattering mobility (cm²/V·s) μ_{LT} total electron mobility (cm²/V·s) μ_n electrical resistivity (Ω·cm) ρ relaxation time along the transverse direction of the ellipsoidal energy surface τ_t τ relaxation time along the longitudinal direction of the ellipsoidal energy surface τ_{LA} relaxation time due to acoustical phonon scattering relaxation time due to ionized impurity scattering τ

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PREFACE

This work was conducted as a part of the Semiconductor Technology Program in the Electronic Technology Division of the National Bureau of Standards (NBS). This program serves to focus NBS efforts to enhance the performance, interchangeability, and reliability of discrete semiconductor devices and integrated circuits through improvements in measurement technology for use in specifying materials and devices in national and international commerce and for use by industry in controlling device fabrication processes. Its major thrusts are the development of carefully evaluated and well documented test procedures and associated technology and the dissemination of such information to the electronics community. Application of the output by industry will contribute to higher yields, lower cost, and higher reliability of semiconductor devices. The output provides a common basis for the purchase specifications of government agencies which will lead to greater economy in government procurement. In addition, improved measurement technology will provide a basis for controlled improvements in fabrication processes and in essential device characteristics.

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The Dopant Density and Temperature Dependence of Electron Mobility and Resistivity in N-Type Silicon

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Sheng S. Li

Abstract: Traditional analysis of electron mobility in *n*-type silicon neglects the effects of electron-electron scattering and scattering anisotropy in the mobility calculations. As a result, theory fails to conform with experiment when dopant density exceeds 2×10^{16} cm⁻³.

In this work, an improved theoretical model for computing mobility and resistivity as functions of dopant density and temperature has been formulated for n-type silicon. The model has been applied to phosphorus-doped silicon for dopant densities from 10^{13} to 10^{19} cm⁻³, and temperatures between 100 and 500 K.

The electron mobility was calculated analytically by appropriately combining lattice, ionized impurity, and neutral impurity scattering contributions. The effect of electron-electron scattering on both lattice and ionized impurity scattering mobilities was incorporated empirically for dopant densities greater than 2×10^{16} cm⁻³. Additionally, the anisotropic scattering effect was also considered in the mobility calculations.

Theoretical calculations of resistivity and ionized donor density were made for phosphorus-doped silicon for temperatures between 100 and 500 K.

Resistivity measurements on seven phosphorus-doped silicon slices with dopant densities from 1.2×10^{14} to 2.5×10^{18} cm⁻³ were carried out for temperatures between 100 and 500 K. Electron mobility at 300 K was deduced from resistivity and junction C-V measurements for dopant densities from 10^{14} to 10^{18} cm⁻³.

Agreement between theory and experiment for both electron mobility and resistivity of phosphorus-doped silicon was within ± 7 percent in the range of dopant densities and temperatures studied.

Key Words: Dopant density; electron mobility; ionized impurity scattering mobility; lattice mobility; neutral impurity scattering mobility; *n*-type silicon; resistivity; scattering mechanisms; temperature.

1. INTRODUCTION

Although a considerable amount of work has been published which deals with electrical properties and mobilities for silicon, it is evident that traditional analysis of electron mobility in *n*-type silicon fails to predict correctly the mobility values when dopant densities exceed 2×10^{16} cm⁻³. The discrepancy may be attributed to the inadequacy of the existing theoretical models in the high dopant density range. For example, the effects of electronelectron collisions and scattering anisotropy on both lattice and ionized impurity scattering mobilities have been neglected in the traditional analysis.

In this work, an improved theoretical model for computing electron mobility and resistivity as functions of dopant density and temperature for phosphorus-doped silicon is described. The calculations cover the range of dopant densities from 10^{13} to 10^{19} cm⁻³, and temperatures between 100 and 500 K. Detailed comparison of the existing scattering theories and mobility formulations for *n*-type silicon is made in section 2 and Appendix A. Calculations of electron mobility and resistivity for phosphorus-doped silicon are described in section 3. Results and discussions are given in section 4. Section 5 presents the conclusions from this work.

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2. SCATTERING MECHANISMS AND MOBILITY FORMULATIONS

In this section, a general review of the existing scattering theories and mobility formulations for *n*-type silicon is given. Scattering processes due to lattice, ionized impurity, and neutral impurity that contribute to the total electron mobility in *n*-type silicon are described. The mobility formulation for each of these scattering processes is described. Quantitative comparison among the mobility values calculated from the different theoretical models for lattice, ionized impurity, and neutral impurity scattering is made. The effects of electron-electron collisions and scattering anisotropy on both lattice and ionized impurity scattering mobilities are discussed.

2.1. Lattice Scattering

Calculations of lattice scattering mobility for *n*-type silicon have been reported by Long [1], Norton *et al.* [2], and others [3,4]. All these calculations are based on the general treatment developed earlier by Herring and Vogt [5] for multivalley semiconductors such as silicon and germanium. The lattice scattering mobility for *n*-type silicon is mainly due to the intravalley acoustical phonon and the intervalley phonon scattering (i.e., the so-called f-type and g-type phonon scattering) [2]. The lattice mobility due to acoustical phonon scattering has been discussed by Brooks [4], using the concept of deformation potential introduced first by Shockley and Bardeen [6], for semiconductors with spherical energy surfaces. The reciprocal relaxation time for this case is [4].

$$\tau_{La}^{-1} = (8\pi^3/h^4) (2m^*)^{3/2} (kT/\rho u_l^2) E_{IC}^2 E^{1/2}$$
(2.1)

which predicts that τ_{La} is proportional to $E^{-1/2}$. The lattice mobility derived from eq (2.1) is* [4]

$$\mu_{La} = \frac{q}{m^*} < \tau_{La} > = \frac{2(2\pi)^{1/2} qh^4 \rho u_{\ell}^2}{3m^* 5/2 (kT)^{3/2} E_{TC}^2}$$
(2.2)

Equation (2.2) predicts that μ_{La} varies as $T^{-1.5}$ for acoustical phonon scattering. For silicon, $(m^*)^{-5/2}$ is replaced by $\frac{1}{3} (m_{\ell}m_{t}^2)^{-1/2} (m_{\ell}^{-1} + 2m_{t}^{-1})$ and $(m_{0}/m^*)^{5/2} = 20.4$; $\rho u_{\ell}^2 = 1.97 \times 10^{12}$ dynes/cm²; $E_{IC} = 12.80$ eV is the deformation potential constant [4]. Lattice mobility described by eq (2.2) assumes that all the scattering events are due to dilation, and that scattering between different ellipsoidal energy surfaces (i.e., the intervalley phonon scattering) has been neglected. The experimental observations of electron mobility for intrinsic silicon, however, shows a stronger temperature dependence of the lattice mobility (i.e., $\mu_{L} \sim T^{-2.3\pm0.2}$) than that predicted by eq (2.2). To correct this discrepancy, Herring [7] has also considered the optical mode and the intervalley phonon scattering for *n*-type silicon. Long [1] has extended the expression to a general case in which there are several intervalley phonons of different energies and scattering strengths and in which the acoustic phonon scattering may be anisotropic. Herring and Vogt [5] have shown that it is legitimate to describe the scattering by a relaxation time tensor diagonal in the principal axes of an energy spheroid. There are two relaxation times for *n*-type silicon, τ_t and τ_{ℓ} .

$$\tau_{\alpha}^{-1} = W_{A\alpha} \left(\frac{E}{kT_{o}}\right)^{1/2} \left(\frac{T}{T_{o}}\right) + \sum_{i} W_{i} \left(\frac{T_{ci}}{T_{o}}\right)^{3/2} \times \left[\frac{(E/kT_{ci} + 1)^{1/2}}{\exp(T_{ci}/T) - 1} + \frac{(E/kT_{ci} - 1)^{1/2}}{1 - \exp(-T_{ci}/T)}\right]$$
(2.3)

^{*}The average relaxation time $\langle \tau \rangle$ for the nondegenerate case is $\langle \tau \rangle = \int_{0}^{\infty} \tau E^{3/2} \exp(-E/kT) dE/\int_{0}^{\infty} E^{3/2} \exp(-E/kT) dE$ where τ is given by (2.1).

The W_A and W_i measure the strength of coupling of the electrons to acoustic and to intervalley phonons, respectively, and the subscript i ranges over all the intervalley phonons of different energies. The subscript α is to be replaced by "t" or " ℓ " depending on the direction relative to the spheroid axis. The temperatures T, T_{ci}, and T_o are, respectively, the temperature at which the relaxation time is to be determined, the characteristic temperature of the ith phonon, and a reference temperature chosen to fix the magnitude of τ . The lattice scattering mobility for *n*-type silicon can be calculated from eq (2.3), by use of the following expression:

$$\mu_{\rm L} = \frac{q}{3} \left[\frac{2 \langle \tau_{\rm t} \rangle}{m_{\rm t}} + \frac{\langle \tau_{\rm l} \rangle}{m_{\rm l}} \right]$$
(2.4)

The procedure for computing μ_L from eq (2.4) is to substitute eq (2.3) into eq (2.4) and to adjust the intervalley coupling constants W_L to give the best fit of the resulting expression to the observed μ_L versus T curve. To simplify the theoretical calculations of μ_L by eqs (2.3) and (2.4), Long [1] has assumed that the possible contributions by all of the various intervalley phonons can be approximated by just two phonons of energies equivalent to temperatures of 630 to 190 K. This approximation is reasonable, since all of the intervalley phonons lie within two rather narrow energy ranges, and these phonons approximately represent average energies of the two ranges. The scattering anisotropy due to the anistropic effective masses m_t and m_t is handled by properly choosing the ratio of coupling constants W_i and W_{AQ} in the mobility calculations. Long [1] has found that choosing the ratio of $W_1/W_{At}^i = 2.0$ and $W_2/W_{At} = 0.15$ yields the best overall fit. The dashed line in figure 1 shows the results of his calculations for temperatures between 100 and 500 K. Norton *et al.* [2] have recently reported a similar calculation (but assuming four intervalley phonons with phonon temperatures $T_1 = 540$ K, $T_2 = 690$ K, $T_3 = 190$ K, and $T_4 = 307$ K) for phosphorus-doped silicon. Their results are also shown in figure 1 by the solid line. It is noted that both curves are in good agreement (within ±3 percent) for temperatures between 100 and 500 K. For a more detailed discussion of their individual treatments, the readers are referred to the original papers by Long [1] and Norton *et al.* [2], respectively. We have used the lattice mobility data of Norton *et al.* [2] for the present mobility calculations.

2.2. Ionized Impurity Scattering

For lightly-doped *n*-type silicon the main contribution to the electron mobility comes from lattice scattering. As the dopant density increases (or temperature decreases), the role of impurity scattering becomes more important. Theories for ionized impurity scattering in semiconductors have been developed by Brooks [4] and Herring [7], Dingle [8], Samoilovich *et al.* [9], and Luong and Shaw [10].

The Brooks-Herring formula is based on the important assumptions that the Born approximation applies, the relaxation time is scalar, the energy surfaces are spherical, electron-electron interactions are negligible, and impurity cell effects can be ignored. The expression for the relaxation time derived from these assumptions, is [7]:

$$T_{\rm I} = \frac{(2m_n^{\star})^{1/2} \varepsilon_{\rm s}^2 E^{3/2}}{\pi q^4 N_{\rm T} G(b)} \times 10^{-6}$$
(2.5)

where $G(b) = \ln (b + 1) - [b/(b + 1)]$,

$$b = \frac{24\pi m_{n}^{*} \epsilon_{s} (kT)^{2}}{q^{2}h^{2}n'} \times 10^{-6}, \text{ and}$$
(2.7)

(2.6)

$$n' = n + n (1 - n/N_{D}), \text{ for } N_{\Delta} = 0$$
 (2.8)

Equation (2.5) predicts that τ_1 is proportional to $E^{3/2}$. The ionized impurity scattering mobility may be derived from eq (2.5) with the result that [7]



Figure 1. Lattice scattering mobility as a function of temperature for n-type silicon calculated by Long [1] (dashed line) and Norton *et al.* [2] (solid line).

$${}^{\mu}\mathbf{I}(BH) = \frac{2^{7/2} \varepsilon_{s}^{2} (kT)^{3/2}}{\pi^{3/2} q^{3} m_{n}^{*1/2} N_{I} G(b)} \times 10^{-2}$$
(2.9)

Equation (2.9) takes no explicit account of any anisotropy in the ion scattering. As a result, it usually overestimates the mobility values, particularly in the high dopant density range where impurity scattering is dominant.

The difficulty in using eq (2.9) for computing the ionized impurity scattering mobility lies in the choice of proper electron effective mass in eqs (2.7) and (2.9) when energy band structure is nonspherical. For silicon, the anisotropic scattering effect comes from electron mass anisotropy (e.g., $m_t = 0.192 \text{ m}_0$ and $m_\ell = 0.98 \text{ m}_0$ [11]) due to the ellipsoidal conduction band structure. Long [14] has made an extensive study of the validity of Brooks-Herring formula for *n*-type silicon for dopant density less than 10^{16} cm^{-3} and temperatures below 100 K. He concluded that if the electron effective mass in eq (2.9) was used as an adjustable parameter, then good agreement between theory and experiment can be obtained. In the present study [12], we have also made a detailed comparison among the theoretical models developed by Brooks-Herring [4,7], Conwell-Weisskopf [13], and Samoilovich *et al.* [9], and have found that the mobility values calculated from these models for *n*-type silicon are generally too large for $10^{13} < N_D < 10^{19} \text{ cm}^{-3}$ and 100 < T < 500 K.[†] To correct this discrepancy, we have made use of the results of Long [14], and Norton *et al.* [2], and obtained a mobility expression, similar to that of eq (2.9), for ionized impurity scattering:

$$\mu_{\rm T} = 7.3 \times 10^{17} \ {\rm T}^{3/2} / {\rm N}_{\rm T} \ {\rm G}({\rm b}_{\rm p}) \,. \tag{2.10}$$

Here $G(b_{\ell})$ is identical to eq (2.6) with the exception that b is replaced by b_{ℓ} , and $m_{\ell}^{2} = 0.98 \text{ m}$ is used in eq (2.7) to obtain b_{ℓ} . The numerical coefficient in eq (2.10) was obtained directly from reference [14] for *n*-type silicon when the anisotropic scattering effect is included. The reader is referred to the original paper [14] for a complete description.

When electron-electron scattering effect is included in eq (2.10) for $N_{\rm D}$ > 2 × 10¹⁶ cm⁻³, the formula appears to yield the best theoretical fit to the measured mobility in the range of dopant density and temperature studied here.

2.3. Neutral Impurity Scattering

Because of the analogy between a neutral donor atom and a hydrogen atom, the mobility for scattering by the neutral donors can be obtained by proper modification of the results for scattering of slow electrons by hydrogen atoms. Erginsoy first predicted a temperature-independent mobility given by [15]:

$$u_{\rm NE} = \frac{2\pi^3 q^3 m_n^*}{5N_N \varepsilon_{\rm s} h^3} \times 10^{-2}$$
(2.11)

This equation fails to predict the temperature dependence of neutral impurity scattering mobility observed for n-type silicon at low temperatures [2]. Sclar [16] sought to improve eq (2.11) by including the possibility of bound states in the electron-hydrogenic impurity scattering problem. He obtained the following expression for the neutral impurity scattering mobility [16]

$$\mu_{\rm N} = 0.82 \ \mu_{\rm NE} \left[\frac{2}{3} \left(\frac{\rm kT}{\rm E_{\rm N}} \right)^{1/2} + \frac{1}{3} \left(\frac{\rm E_{\rm N}}{\rm kT} \right)^{1/2} \right], \qquad (2.12)$$

$$E_{\rm N} = 1.136 \times 10^{-19} \, ({\rm m}_{\rm n}^*/{\rm m}_{\rm o}) \, (\varepsilon_{\rm o}^{\prime}/\varepsilon_{\rm s}^{\prime})^2$$
 (2.13)

+For details see Appendix A.



Figure 2. Neutral impurity scattering mobility as a function of donor density computed from eq (2.11) (due to Enginsoy) - eq (2.12) (due to Sclar).

and $\mu_{\rm NF}$ is given by eq (2.11).

Equation (2.12) predicts that μ_N varies as $T^{1/2}$ for kT above the binding energy, E_N . The experimental data given by Norton *et al.* [2] for *n*-type silicon show such a dependence up to 50 K. Our mobility and resistivity calculations using eqs (2.11) and (2.12) show that the latter produces a better fit with the experimental data than the former. For comparison, the neutral impurity scattering mobilities computed from eqs (2.11) and (2.12) are shown in figure 2 for T = 300 K. Note that the mobility values predicted by eq (2.11) are somewhat smaller than those of eq (2.12).

2.4. Effect of Electron-Electron Scattering

The mobility formula given in eq (2.10) neglects the effect of electron-electron (e-e) scattering on the ionized impurity scattering mobility. Although e-e scattering does not affect the current density directly since it cannot alter the total momentum, it tends to randomize the way in which this total momentum is distributed among electrons with different energy. When the scattering mechanism is such as to lead to a nonuniform distribution, e-e scattering gives rise to a net transfer of momentum from electrons which dissipate momentum less efficiently to those which dissipate more efficiently, resulting in an overall greater rate of momentum transfer and lower mobility.

On the basis of the above argument, it is obvious that the size of the effect of e-e scattering on the mobility is a function of the energy dependence of the relaxation time. Thus, for neutral impurity scattering where the relaxation time is independent of energy, the mobility is not affected by e-e scattering. Ionized impurity scattering would be expected to be much more affected than lattice scattering since in the former case $\tau_{\rm I}$ is proportional to ${\rm E}^{3/2}$, while in the latter it is proportional to ${\rm E}^{-1/2}$.

Luong and Shaw [10] have analyzed the effect of e-e scattering on the ionized impurity mobility using a single-particle-like approximation from the time-independent Hartree-Fock theory. They have shown that with the correction for e-e scattering, the Brooks-Herring formula is reduced by a factor which can be expressed in closed form as [10]

$$\mu_{\rm I}^{"} = (1 - e^{-n/N}I) \mu_{\rm I}$$
 (2.14)

where N_I is the ionized impurity density, n is the electron density, and μ_I is given by eq (2.10). For uncompensated *n*-type silicon, the density of ionized donor impurities, N_I , is equal to the density of conduction electrons, n. Thus, eq (2.14) reduces to

$$\mu_{\rm T}^{\prime\prime} = (1 - e^{-1}) \ \mu_{\rm T} = 0.632 \ \mu_{\rm T} \tag{2.15}$$

The factor in eq (2.15) is in good agreement with a previous prediction [17] based on the Boltzmann theory. For *n*-type silicon, the effect of e-e scattering on the ionized impurity scattering becomes important for $N_D > 2 \times 10^{16} \text{ cm}^{-3}$, as will be discussed later.

The effect of e-e scattering on the lattice mobility has also been discussed in several classical papers [4,18,19]. It can be shown [18,19] that e-e scattering reduces the lattice scattering mobility by a maximum of 12 percent. This factor will be used in the present calculations.

3. CALCULATIONS OF ELECTRON MOBILITY AND RESISTIVITY IN N-TYPE SILICON

3.1. Electron Mobility Calculations

We now discuss the mobility calculations for *n*-type silicon in the range of dopant density from 10^{13} to 10^{19} cm⁻³ and temperature from 100 to 500 K.

The combined mobility due to both lattice and ionized impurity scattering contributions can be calculated according to the mixed-scattering formula [18]:

$$\mu_{LI} = \mu_{L} \left[1 + X^{2} \left(\text{CiX cosX} + \text{sinX} \left(\text{SiX} - \frac{\pi}{2} \right) \right]$$
(3.1)

where $\boldsymbol{\mu}_{T}$ is the lattice mobility,

$$X^2 = 6\mu_L/\mu_T$$
, (3.2)

and μ_{T} is given by eq (2.10).

CiX and SiX are the cosine and sine integrals of X, respectively. Note that eqs (3.1) and (3.2) are applicable for donor densities less than 2×10^{16} cm⁻³ where the effect of e-e scattering is negligible. For dopant densities greater than 2×10^{16} cm⁻³, the effect of e-e scattering is incorporated empirically in eq (3.2) as follows:

(i) High dopant density range
$$(2 \times 10^{17} < N_p < 10^{19} \text{ cm}^{-3})$$
.

In this dopant density range, experimental evidence indicates that the full effect of e-e scattering should be taken into account in the mobility calculations, and eq (3.2) is replaced by:

$$X''^{2} = 6 \mu_{T}''/\mu_{T}'' , \qquad (3.3)$$

where

$$\mu_{\rm L}^{\prime\prime} = 0.88 \ \mu_{\rm L},$$
 (3.4)

and,

 $\mu_{\rm T}^{\prime\prime} = 0.632 \ \mu_{\rm T}. \tag{3.5}$

(ii) Intermediate dopant density range $(2 \times 10^{16} \le N_p \le 2 \times 10^{17} \text{ cm}^{-3})$.

In this dopant density range, the effect of e-e scattering on both lattice and ionized impurity scattering mobilities is increased gradually with increasing dopant density. To obtain the best fit to the measured mobility at 300 K in this transition range, the mobility reduction factors $R(N_D)$ and $S(N_D)$, for both μ_I and μ_I were derived empirically, assuming a linear dependence on the donor density. The results are given by:

$$\mu_{\rm L}^* = R(N_{\rm D}) \ \mu_{\rm L}, \tag{3.6}$$

where

$$R(N_{\rm D}) = 1.013 - 6.62 \times 10^{-19} \times N_{\rm D}$$
(3.7)

and

$$\mu_{I}' = S(N_{D}) \mu_{I}, \qquad (3.8)$$

where

$$S(N_{\rm D}) = 1.04 - 2.04 \times 10^{-18} \times N_{\rm D}$$
 (3.9)

The mobility ratio in eq (3.2) is now replaced by

$$X'^{2} = 6 \mu_{\rm L}'/\mu_{\rm T}'$$
(3.10)

Note that the mobility reduction factors, $R(N_D)$ and $S(N_D)$, in eqs (3.7) and (3.9) decrease linearly from 1 to 0.88 and 0.632, respectively, as the dopant density, N_D , increases from 2 × 10¹⁶ to 2 × 10¹⁷ cm⁻³.

Equations (3.1) through (3.10) allow the calculations of μ_{LT} for $10^{13} \leq N_D \leq 10^{19}$ cm⁻³, and 100 < T < 500 K. When neutral impurity scattering is included, the total electron mobility may be computed from the expression

$$\mu_{n} = (\mu_{LI}^{-1} + \mu_{N}^{-1})^{-1}$$
(3.11)

where μ_{LI} is given by eq (3.1) and μ_{N} is the mobility due to neutral impurity scattering as given in eq (2.12). A sum of the reciprocal mobilities for this case is expected to yield a considerably better approximation than it does for the reciprocal sum of μ_{L} and μ_{J} because neutral impurity scattering, being energy independent, does not affect any contributions from μ_{J} and μ_{J} .

3.2. Ionization of the Donor Impurity

In this section, formulations are given for computing the ionized donor density (or electron density) as a function of the total donor density in uncompensated *n*-type silicon. In order to compute the electron mobility and resistivity, it is necessary to know the amounts of ionized and neutral impurity atoms so that their scattering contributions can be calculated.

The ionized donor densities for *n*-type silicon were computed by solving the charge balance equation for the Fermi energy by an iteration procedure. Since the minority carrier density (i.e., hole density in *n*-type silicon) is negligibly small for this case, the charge balance equation is simply

$$n \approx N_{\rm D}^{+} \tag{3.12}$$

where

$$N_{D}^{+} = \frac{N_{D}}{1 + 2 \exp[(E_{F} - E_{C} + E_{D})/kT]}$$
(3.13)

and the electron density, n, is given by [20]

$$n = N_C / [exp(E_C - E_F)/kT + 0.27], \text{ for } E_F < 1.3 kT$$
 (3.14)

where $N_{C} = 2 \left[\frac{2\pi m_{d}^{*} kT}{h^{2}} \right]^{3/2}$ is the effective density of conduction band states (N_{C} = 3.22 × 10¹⁹ cm⁻³ for *n*-type silicon at 300 K). The temperature dependence of the density of states effective mass was taken into account in accordance with the results of Barber [11].

Experimental evidence exists which shows that the donor ionization energy, $\varepsilon_{\rm D}$, is not constant, but decreases with increasing dopant density. Hall coefficient measurements by Pearson and Bardeen [21] and more recently by Penin *et al.* [22] in heavily-doped silicon from 4 to 300 K show no evidence of an ionization energy at impurity densities greater than 3×10^{18} cm⁻³. For *n*-type silicon doped with phosphorus impurities, the dependence of donor ionization energy on the dopant density is [18]

$$\varepsilon_{\rm D} = \varepsilon_{\rm D}({\rm o}) - \alpha \, N_{\rm D}^{-1/3} \tag{3.15}$$

where $\varepsilon_{\rm D}({\rm o}) = 0.045$ eV is the ionization energy of the phosphorus donor; with $\alpha = 3.1 \times 10^{-8}$, eq (3.15) gives a zero ionization energy for N_D = 3 × 10¹⁸ cm⁻³.

3.3. Resistivity Analysis

Measurements of resistivity in silicon have been reported by previous investigators [23-35]. Irvin [25] first showed complete resistivity versus dopant density curves for both n- and ptype silicon at 300 K, using mostly previously published data. Recently Mousty *et al.* [26] reported the resistivity versus phosphorus density in n-type silicon. The electrical properties of heavily-doped silicon were also reported by Chapman *et al.* [28]. Most of these efforts focused on resistivity measurements near room temperature. A theoretical analysis of the resistivity as a function of dopant density for n-type silicon has been reported by Rode [3] and Norton *et al.* [2]; their calculations of resistivity were also confined to room temperature. In this work, we have extended the theoretical calculations of resistivity as a function of dopant density for *n*-type silicon for $10^{13} \le N_n \le 10^{19}$ cm⁻³, and $100 \le T \le 500$ K.

The resistivity is calculated from the expression

$$\rho = \frac{1}{qn\mu_n} \tag{3.16}$$

If both ρ and n are measured independently, then the electron mobility may be deduced from eq (3.16). On the other hand, if μ and n are computed from the theoretical expressions discussed above, it is then possible to compare between theoretically computed and experimentally measured resistivity. We shall discuss this further in section 4.2.

4. RESULTS AND DISCUSSIONS

In this section, calculations of partial mobilities, electron mobility, electron density, and resistivity as functions of dopant density and temperature, based on the theoretical formulas discussed in the preceding section, are described. Results of the resistivity measurements and electron mobility data for phosphorus-doped silicon are presented.

4.1. Electron Mobility vs. Dopant Density and Temperature

The mobility formulas used in the present calculations are listed in table 1. As noted in this table the mobility calculations carried out in three distinct dopant density ranges are based on our analysis of the electron mobility data versus dopant density at 300 K and the resistivity data for phosphorus-doped silicon taken at temperatures between 100 and 500 K. The mobility formulas in column (I) of table 1 may be referred to as the traditional mobility formulations which neglect the effect of electron-electron scattering. The mobility calculations from these formulas for *n*-type silicon are in good agreement (within ±5 percent) with experimental data for dopant densities up to 2×10^{16} cm⁻³, but for greater dopant densities the calculated mobility is larger than the measured mobility. By including the effect of e-e scattering in the mobility formulas shown in columns (II) and (III), we were able to bring into accord (within ±5 percent) the theoretical calculations and the experimental data at 300 K for dopant densities between 10^{13} and 10^{19} cm⁻³.

Figure 3 shows the electron mobility as a function of donor density computed at 300 K, along with experimental data for phosphorus-doped silicon. The solid dots are taken from the mobility data of Mousty et al. [26], and Baccarani and Ostoja [29], corrected to 300 K, and the open circles are data obtained by Buehler et al. [30,31] on processed phosphorus-doped silicon slices. A planar four-probe structure was used for resistivity measurements [30] and a diffused diode near the four-probe test structures was used for junction C-V measurements of donor density [31]. The theoretical calculations (curve 3) are within ± 5 percent of the experimental data for dopant densities from 10^{14} to 10^{19} cm⁻³. For comparison, the Irvin mobility curve (curve 2) which was calculated from the Caughey and Thomas [32] empirical formula for *n*-type silicon is also shown by a dashed line in figure 3. To illustrate the important effect of e-e scattering, we have also shown in figure 3 the theoretical calculations of electron mobility as a function of dopant density (see curves 1 and 4) with and without inclusion of electron mobility as a function of dopant density (see curves 1 and 4) with and without inclusion of e-e scattering effect over the entire range of dopant density from 10^{13} to 10^{19} cm⁻³. It is clearly demonstrated that the mobility values predicted in curve 1 are smaller than the measured mobility for N_D $\leq 2 \times 10^{17}$ cm⁻³ when e-e scattering is included in this dopant density range. On the other hand, the mobility values predicted in curve 4 are larger than the measured mobility for N_D $\geq 2 \times 10^{16}$ cm⁻³ when e-e scattering is neglected. Thus, a transition region (i.e., $2 \times 10^{16} \leq N_D \leq 2 \times 10^{17}$ cm⁻³) exists in which the effect of e-e scattering increases gradually with increasing dopant density. The mobility formulas in table 1 were also applied to compute the electron mobility as a function of dopant density for temperatures between 100 and 500 K. The results are displayed in figures 4 and 5. Mobility was not determined directly at temperatures other than 300 K so no attempt has been made to compare theory with experiment.

4.2. Resistivity vs. Dopant Density and Temperature

Electrical resistivity as a function of dopant density for phosphorus-doped silicon was calculated using eq (3.16). Values of μ_n were obtained from the results of section 4.1., and the electron density was computed by Solving eqs (3.12) through (3.14) using the iteration TABLE 1 — Formulas for Computing Electron Mobility in n-type Silicon for 100 < T < 500 K.

(1) $10^{13} \le N_{\rm D} \le 2 \times 10^{16} {\rm cm}^{-3}$	(II) $2 \times 10^{16} \le N_D \le 2 \times 10^{17} \text{ cm}^{-3}$	(III) $2 \times 10^{17} \le N_{\rm D} \le 10^{19} {\rm cm}^{-3}$
 (1) Lattice Mobility [2]: μL Values of μL are obtained from Norton <i>et al.</i> [2] (la) (See figure 1 of this paper.) 	(1) Lattice Mobility: μ_{L}^{i} $\mu_{L}^{i} = R(N_{D}) \cdot \mu_{L} \cdot (1b)$ where $R(N_{D}) = (1.013 - 6.62 \times 10^{-19} \times N_{D})$	(1) Lattice Mobility: $\mu_{L}^{"}$ $\mu_{L}^{"} = 0.88 \ \mu_{L} \cdots \cdots \cdots \cdots \cdots (lc)$
(2) <u>Ionized Impurity Mobility</u> [10]: μ_{I} $\mu_{I} = 7.3 \times 10^{17} \times T^{3/2}/N_{I} G(b_{g}) \ldots \ldots \ldots \ldots (2a)$ where $G(b_{g}) = 2n(b_{g} + 1) - b_{g}/(b_{g} + 1)$ $b_{g} = 1.52 \times 10^{15} \times T^{2}/n^{1}$	(2) Ionized Impurity Mobility: μ_{I}^{\prime} $\mu_{I}^{\prime} = S(N_{D}) \cdot \mu_{L} \cdot \cdots \cdot \cdot \cdot \cdot \cdot \cdot (2b)$ where $S(N_{D}) = (1.04 - 2.04 \times 10^{-18} \times N_{D})$	(2) Ionized Impurity Mobility: $\mu_{I}^{"}$ $\mu_{I}^{"} = 0.632 \ \mu_{I} \cdots \cdots (2c)$
(3) Mixed Scattering Formula for μ_{LI} [15]: $\mu_{LI} = \mu_L f(X) \cdots \cdots$	(3) Mixed Scattering Formula for μ_{LI}^{i} $\mu_{LI}^{i} = \mu_{L}^{i} f(X^{i}) \cdots \cdots \cdots \cdots (3b)$ where $X^{i}^{2} = 6\mu_{L}^{i}/\mu_{I}^{i}$	(3) Mixed Scattering Formula for $\mu_{LL}^{"}$ $\mu_{LL}^{"} = \mu_{L}^{"} f(X^{"}) \cdot \cdot \cdot \cdot \cdot \cdot \cdot (3c)$ where $X^{"2} = 6\mu_{L}^{"}/\mu_{T}^{"}$
(4) Neutral Impurity Mobility [2]: $\mu_{\rm N}$ $\mu_{\rm N} = (3 \times 10^{20}/{\rm N}_{\rm N}) \cdot (0.1495 \ T^{1/2} + 1.482/T^{1/2}) \dots (4a)$	<pre>(4) Neutral Impurity Mobility: µ_N same as (4a) (4b)</pre>	<pre>(4) Neutral Impurity Mobility: µN same as (4a) (4c)</pre>
(5) Total Electron Mobility: μ_n $\mu_n = (1/\mu_{LI} + 1/\mu_N)^{-1} \cdots \cdots$	(5) Total Electron Mobility: μ_{n} $\mu_{n} = (1/\mu'_{LI} + 1/\mu_{N})^{-1} \dots (5b)$	(5) Total Electron Mobility: μ_n $\mu_n = (1/\mu'_{LI} + 1/\mu_N)^{-1} \cdot \cdot \cdot (5c)$

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Figure 3. Electron mobility versus total donor density for *n*-type silicon at 300 K. (Curve 1 is the theoretical calculation with e-e scattering included for $10^{13} < N_D < 10^{19}$ cm⁻³, curve 2 is the Irvin curve calculated from the Caughey and Thomas empirical formula [30], curve 3 is the exact theoretical calculation using mobility formulas in Table 1, curve 4 is the theoretical calculation with e-e scattering neglected. Open circles are NBS data [27], and solid dots are from Mousty *et al.* [24] for phosphorus-doped silicon.)



Figure 4. Electron mobility of *n*-type silicon versus temperature for dopant densities from 10^{13} to 5×10^{18} cm⁻³.





procedure mentioned in section 3.2. The results are displayed in figures 6 through 10.

In figure 6, the theoretical curves are shown for the percent ionization of phosphorus atoms versus total phosphorus density for temperatures between 100 and 500 K. The electron density was obtained from eq (3.12), which is a valid approximation for the uncompensated case. Figure 7 shows the resistivity versus donor density for *n*-type silicon at 300 K; the solid line is our theoretical calculation, and the dashed line is the Irvin curve [25]. The calculated resistivity is 5 to 10 percent smaller than the resistivity given by the Irvin curve for the same value of dopant density; this is consistent with recently published resistivity data [26,31].

In order to compare theory with experiment for temperature other than 300 K, resistivity measurements were made between 100 and 500 K on seven phosphorus-doped silicon wafers with densities from 1.2×10^{14} to 2.5×10^{18} cm⁻³.

The resistivity measurements were performed using a planar four-probe test structure which was designed for bulk resistivity measurements and was fabricated using the bipolar transistor process. The test cells used for the resistivity measurements were obtained from the same silicon wafers fabricated for the mobility measurements at 300 K (see figure 3). For temperature dependent measurements, the test cell containing the four-probe structure was mounted on a TO-5 header, and a temperature-sensing diode was also mounted next to the cell for measuring the temperature. The TO-5 header was then mounted inside a specially-designed cryostat where temperatures can be varied from -191 to 400° C with a maximum heating rate of 7 K/s [32].

Figure 8 shows the plot of resistivity as a function of temperature for phosphorus-doped silicon with dopant densities from 1.2×10^{14} to 2.5×10^{18} cm⁻³; the solid lines are the theoretical calculations and the solid dots are the measured resistivity. Figure 9 displays the calculated resistivity versus temperature for dopant densities from 5×10^{13} to 10^{19} cm⁻³ in more regular steps. Figure 10 shows the calculated resistivity curves as a function of dopant density for temperatures between 100 and 500 K. The results show that the resistivity depends strongly on temperature for N_D < 10^{16} cm⁻³ where lattice scattering is dominant. However, the resistivity is nearly independent of temperature for N_D > 10^{18} cm⁻³ where mixed scattering prevails.

5. CONCLUSIONS

An improved theoretical model has been formulated for computing electron mobility in *n*-type silicon as functions of dopant density and temperature. In addition to considering the contributions from scattering by lattice phonons, ionized impurities, and neutral impurities, this model takes into account the effect of electron-electron scattering on both lattice and ionized impurity scattering mobilities for dopant densities greater than 2×10^{16} cm⁻³.

From this study, it was found that the influence of e-e scattering is negligible for $N_D \leq 2 \times 10^{16} \text{ cm}^{-3}$, but is significant for $N_D \geq 10^{17} \text{ cm}^{-3}$. To allow a smooth change in the calculated mobility values across the boundaries of the transition region (i.e., $2 \times 10^{16} \leq N_D \leq 2 \times 10^{17} \text{ cm}^{-3}$), the effect of e-e scattering is assumed to increase linearly with dopant density in this region. The theoretical predictions, based on such an assumption, are within ±5 percent of the measured mobilities for $10^{13} \leq N_D \leq 10^{19} \text{ cm}^{-3}$, and T = 300 K.

Resistivity analysis for phosphorus-doped silicon shows that for dopant densities less than 3×10^{18} cm⁻³, the calculated resistivity values are within ±7 percent of the experimental data for temperatures between 100 and 500 K.









Figure 8. Resistivity versus temperature for seven phosphorus-doped silicon slices. (Solid lines are the theoretical calculations and dots are the experimental data.)







Figure 10. Theoretical calculations of resistivity versus total donor density for n-type silicon with temperature as a parameter (100<T<500 K).

APPENDIX A: COMPARISON OF THE EXISTING MODELS FOR IONIZED IMPURITY SCATTERING

In addition to the Brooks-Herring (BH) mobility formula already discussed in section 2.2. of the main text, we now proceed to discuss other existing models for computing the ionized impurity scattering mobility in *n*-type silicon. These include the Conwell-Weisskopf (CW) formula [13] and the formulas derived more recently by Samoilovich, Korenblit, and Dakhovskii (SKD) [9].

(i) Conwell-Weisskopf (CW) Formula:

Using the Born approximation and assuming that the impurity potential is a bare Coulomb potential (i.e., $V(r) = \frac{q}{\epsilon_s r}$), Conwell and Weisskopf derived a mobility expression which reads [13]:

$$\mu_{I(CW)} = \frac{128(2\pi)^{1/2} \epsilon_{s}^{2} k^{3/2}}{q^{3} m_{n}^{*1/2} N_{I}} \left\{ \ln \left[1 + \left(\frac{12\pi \epsilon_{s} kT^{2}}{q} \right)^{2} N_{I}^{-2/3} \right] \right\}^{-1}$$
$$= \frac{4.55 \times 10^{17} T^{3/2}}{N_{I}} \left\{ \ln \left[1 + \frac{4.42 \times 10^{8} T^{2}}{N_{I}^{2/3}} \right] \right\}^{-1}$$
(A.1)

The numerical values in the brackets of eq (A.1) are obtained by substituting $m^* = 0.26 \text{ m}$ and $\varepsilon = 11.7 \times 8.852 \times 10^{-14} \text{ F/cm}$ in the above equation. The theoretical values of μ_{I} calculated from eq (A.1) are shown in figure A.1 (see curve 4).

(ii) The SKD Formula:

Samoilovich *et al.* [9] have derived a theoretical model for computing ionized impurity scattering mobilities in *n*-type silicon taking into account the effect of scattering anisotropy. The results of their mobility formulations can be summarized as follows.

The average relaxation times along the transverse and longitudinal axis of the ellipsoidal conduction band valley of silicon are given, respectively, by [2]:

$$\langle \tau_{t} \rangle = 5.48 \times 10^{11} (g_{1} + 1) / \{ N_{I} \times [\ln (b_{l}) - 2.34 + 7.88/b_{l}] \}$$
 (A.2)

and,

$$\tau_{\ell} > = 1.98 \times 10^{12} (g_0 + 1) / \{N_I \times [\ln(b_{\ell}) - 1.75 + 4.64/b_{\ell}]\}$$
 (A.3)

where

$$g_1 = 0.03 \times [\log_{10} (b_0) - 1]$$
 (A.4)

$$g_{o} = 0.192 - 0.335/log_{10} (b_{o})$$
 (A.5)

$$b_{0} = 1.52 \times 10^{15} T^{2}/n'$$
 (A.6)

$$n' = n + n \cdot (1 - n/N_{D}), \text{ for } N_{A} = 0$$
 (A.7)

The mobility is then computed from the following expression:

$$\mu_{I(SKD)} = \frac{q}{3} \quad \left(\frac{2 \langle \tau_{t} \rangle}{m_{t}} + \frac{\langle \tau_{\ell} \rangle}{m_{\ell}}\right) = 5.86 \times 10^{8} (10.4 \langle \tau_{t} \rangle + 1.02 \langle \tau_{\ell} \rangle)$$
(A.8)

Here $\langle \tau_{2} \rangle$ and $\langle \tau_{2} \rangle$ are the Maxwellian average relaxation time components given by eqs (A.2) and (A.3), respectively. The mobility versus dopant density, as calculated from eq (A.8),



Figure A-1. Ionized impurity scattering mobility versus total donor density as computed from different theoretical models at 300 K. (Curve 1 is calculated from eq (2.10), curve 2 from eq (2.9), curve 3 from eq (A-8), and curve 4 from eq (A-1).)

is shown in figure A.1 (i.e., curve 3). For comparison, the mobility curves calculated from the Brooks-Herring formula (i.e., eq (2.9)) and the modified formula (i.e., eq (2.10)) discussed in the main text are also included in figure A.1 (see curves 2 and 1). Note that corrections due to e-e scattering for $N_D > 2 \times 10^{16}$ cm⁻³ have also been taken into account for all four curves shown in figure A.1. The results show that for $N_D < 10^{18}$ cm⁻³ the mobility values predicted by the three existing models are in reasonable agreement (within ±20 percent), but are 25 to 50 percent larger than those predicted by the modified formula (i.e., eq (2.10)). However, for $N_D > 10^{18}$ cm⁻³, the mobility values calculated by both the SKD and BH formulas are considerably larger (about 50 to 100 percent) than those from eq (2.11).

In conclusion, the present results suggest that the mobility formulations for ionized impurity scattering derived by Conwell-Weisskopf, Brooks-Herring, and Samoilovich *et al.* appear to overestimate the mobility for *n*-type silicon, particularly for $N_D > 10^{18} \text{ cm}^{-3}$. One possible reason for this discrepancy may be attributed to the anisotropic scattering effect resulting from electron mass anisotropy in *n*-type silicon, as pointed out in the main text. For *p*-type silicon where hole effective masses are nearly isotropic, the above mentioned difficulty would not be expected to occur.

In this appendix, we calculate two important physical parameters which are relevant to the mobility calculations discussed in the main text and Appendix A. These two parameters are the dielectric screening length, R₁, and the degeneracy temperature, T₁. For the sake of simplicity, we consider here the case of phosphorus-doped silicon in which one extra electron is provided by each phosphorus donor atom which then becomes positively charged when ionized. Let n be the density of electrons in the conduction band, and V(r) the electrostatic potential. In the presence of the self-consistent field due to V(r), the ordinary space-independent Fermi energy, E_f, must be replaced by E_F + qV(r), and V(r) can be obtained by solving Poisson's equation. The result is given by [7]:

1

$$V(r) = \left(\frac{q}{\varepsilon_{r}}r\right) \exp\left(-r/R_{n}\right)$$
(B.1)

where

$$R_{n} = \left(\frac{1}{q}\right) \left(\frac{\varepsilon_{s}^{kT}}{4\pi n}\right)^{1/2}$$
(B.2)

For n-type silicon, eq (B.2) reduces to

$$R_{\rm p} = 23.6 \ {\rm T}^{1/2} \ {\rm n}^{-1/2} \ ({\rm cm})$$
 (B.3)

which shows that the dielectric screening length is inversely proportional to the square root of the electron density. Equation (B.3) was used to calculate the dielectric screening length versus dopant density for *n*-type silicon for temperatures between 100 and 500 K. The results are shown in figure B.1. For comparison, the interatomic spacing of the silicon lattice is also included in this figure. Note that the dielectric screening of conduction electrons may be considered "complete" if R >> d_{si}, where d_{si} is the spacing of silicon atoms. For *n*-type silicon, this condition is satisfied for N_D <^{si} × 10¹⁸ cm⁻³ and T > 100 K. Thus, calculations of ionized impurity scattering mobility by the Brooks-Herring formula, as discussed in the main text, should be valid for N_D < 3×10^{18} cm⁻³ and T > 100 K. However, for higher temperatures (e.g., T ≥ 250 K), the validity of the Brooks-Herring formula may be extended to N_D $\sim 10^{19}$ cm⁻³, since the dielectric screening length also increases with increasing temperature.

The degeneracy temperature of the electron system in *n*-type silicon is calculated from the following expression [7]:

 $T_{d} = \left(\frac{h^{2}}{8m_{p}^{*}k}\right) \left(\frac{3n}{8\pi}\right)^{2/3}$ (B.4)

Equation (B.4) was used to compute the degeneracy temperature as a function of electron density for *n*-type silicon, and the result is shown in figure B.2. The curve may serve as a demarcation line which separates the degenerate region (i.e., above the curve) from the nondegenerate region (i.e., below the curve) as shown in the figure. This plot is useful for identifying the validity of the statistics used in the mobility calculations. For example, at T = 100 K, nondegenerate statistics may be used in the mobility calculations for dopant densities up to 3×10^{18} cm⁻³ and this may be extended to 7×10^{18} cm⁻³ for T = 300 K.



Figure B-1. Dielectric screening length versus donor density for 100<T<500 K for phosphorus-doped silicon.



Figure B-2. Degeneracy temperature as a function of electron density for n-type silicon.

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16. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.) Traditional analysis of electron mobility in n-type silicon neglects the effects of electron-electron scattering and scattering anisotropy in the mobility calculations. As a result, theory fails to conform with experiment when dopant density exceeds 2 × 10 ¹⁶ cm ⁻³			
In this work, an improved theoretical model for computing mobility and resistivity as functions of dopant density and temperature has been formulated for <i>n</i> -type silicon. The model has been applied to phosphorus-doped silicon for dopant densities from 10^{13} to 10^{19} cm ⁻³ , and temperatures between 100 and 500 K. The electron mobility was calculated analytically by appropriately combining lattice, ionized impurity, and neutral impurity scattering contributions. The effect of electron electron scattering on both lattice and ionized impurity scattering mobilities was in- corporated empirically for dopant densities greater than 2×10^{16} cm ⁻³ . Additionally, the anisotropic scattering effect was also considered in the mobility calculations. Theoretical calculations of resistivity and ionized donor density were made for phosphorus-doped silicon for temperatures between 100 and 500 K. Resistivity measurements on seven phosphorus-doped silicon slices with dopant den- sities from 1.2×10^{14} to 2.5×10^{18} cm ⁻³ were carried out for temperatures between 100 and 500 K. Electron mobility at 300 K was deduced from resistivity and junction C-V measurements for dopant densities from 10^{14} to 10^{18} cm ⁻³ .			

Agreement between theory and experiment for both electron mobility and resistivity of phosphorus-doped silicon was within ±7 percent in the range of dopant densities and temperatures studied.

17. KEY WORDS (six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons) Dopant density; electron mobility; ionized impurity scattering mobility; lattice mobility; neutral impurity scattering mobility; n-type silicon; resistivity; scattering mechanisms; temperature.

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