Resolution of the Scaling Exponent Puzzle for Weakly Compensated Crystalline Silicon and Germanium Metal-Insulator Systems

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Using a classical theory for ionized impurity scattering, it is demonstrated that in the degenerate regime the conductivity scales as $\sqrt{\epsilon_F}$ where the Fermi energy is measured with respect to the mobility edge. The approach, a special case of alloy theory, explains the conductivity scaling exponent $s = \frac{1}{2}$ observed for weakly compensated, doped crystalline Si and Ge. The results explain the breadth of scaling range and suggest how to obtain a consistent picture of the scaling of the mobility, diffusion coefficient, and Hall coefficient.

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One of the important unresolved issues concerning the metal-insulator transition (MIT) in weakly compensated doped Si and Ge is an explanation for the scaling exponent s of the conductivity $\sigma(n, T \to 0) = \sigma_0(n/n_c - 1)^s$ where s has been found to be close to 0.50 for Si:P [1], Si:As [2], Si:Sb [3], Si:B [4], Ge:Sb [5], Ge:As [6], and Ge:Ga [7]. Of particular note are the Si:P uniaxial stress and neutron-transformation doped (NTD) ^{70}Ge:Ga results that approached n_c more closely than other studies, namely $1.0001n_c$ for Si:P and 1.0004 for Ge:Ga. These two studies were also carried to lower T [3 mK for Si:P, 20 mK for Ge:Ga] than the other studies. The other systems, with minor corrections to n_c, also show $s \sim 0.50$ and support the notion of a universal [8] exponent $s = \frac{1}{2}$. In contrast, the amorphous semiconductor-metal alloy systems all show $s \sim 1.0$, which is in agreement with the Wegner [9] prediction $\sigma(0) \propto (E_F - E_c)^{(d-2)\nu}$ $[d = 3, \nu = 1]$ and the Abrahams *et al.* [10] scaling prediction from the $\beta(g)$ function approach. There have now been at least six different proposals [11–16] to explain the $s = 0.5$ result, but none of them have been widely accepted. While it has been clear that both disorder and electron-electron (e-e) interactions are important features of the MIT in these systems it hasn't been possible to proceed beyond perturbation results that are first order in the disorder. Although the experimental results give strong evidence for the Altshuler-Aronov [17] diffusive correction $\delta\sigma_D(n, T) = m(n)\sqrt{T}$ at finite T the role of e-e interactions at $T = 0$ is less obvious. The dominant low temperature scattering mechanism for doped semiconductors and dilute alloy systems, ionized impurity scattering (IIS), has not yet played a central role in interpreting MIT transport results. The field of IIS, with its complications and complexities, has been comprehensively reviewed by Chattopadhyay and Queisser [18]. In this paper IIS, a classical theory [19–21] well known for five decades in semiconductor physics, is shown to yield $s = \frac{1}{2}$. This robust result is independent of the form of the density of states (DOS) above the mobility edge at E_c and depends only on the system being sufficiently degenerate $[(E_F - E_c)/kT \gg 1]$. The approach assumes the random potential and Anderson localization [22], which produce the mobility edge at E_c, and incorporates the two-component model with a density n_l of localized electrons below E_c and a density n_a of itinerant electrons above E_c such that $n_a + n_l = n = N_d - N_a$. Simple theoretical notions and the Hall coefficient results argue that $n_a \to 0$ as $n \to n_{c+}$.

A general expression for $\sigma(n, T)$ given by Mansfield [23], valid for arbitrary degeneracy which can be utilized for scattering from a random distribution of ionized impurities, is

$$\sigma(T) = (2e^2/3m^* kT) \int_{E_c}^{\infty} \tau N(E)(E - E_c) f(1 - f)\, dE, \tag{1}$$

where his DOS $N(E) = 4\pi(2m^*)^{3/2}(E - E_c)^{1/2}/h^3$ was intended for the host semiconductor conduction band $[E_c = E_{\mathrm{CB}}]$. Here E_c refers to the mobility edge of the impurity band, which is well below E_{CB} in most of the many-valley semiconductors. f is the Fermi function. It is straightforward to show for $E_F - E_c/kT \gg 1$ Eq. (1) leads to the standard Boltzmann result $\sigma_B = ne^2\tau(E_F)/m^*$ where $n = \int_{E_c}^{\infty} N(E) f\, dE$. For the present case an arbitrary DOS $N(E) = C[(E - E_c)/E_0]^p$ will be employed, although the same basic result is found if one adds $N(E_c)$ to $N(E)$. For IIS the collision rate $1/\tau = N_i v\langle\sigma\rangle$, where N_i is the density of ionized impurities, $v = \hbar k/m^*$, and the angle averaged cross section $\langle\sigma\rangle = (4\pi/k^2)\sum_l (l + 1)\sin^2(\delta_l - \delta_{l+1})$. The phase shifts δ_l are restricted by the Friedel [24] sum rule $Z\pi/2 = \sum_l (2l + 1)\delta_l$. The number of itinerant electrons above E_c is given by $n_a = \int_{E_c}^{\infty} N(E) f\, dE = CE_0(kT/E_0)^{p+1} F_p(\eta^*)$ where the Fermi integral $F_p(\eta^*) = \int_0^{\infty} \eta^p f\, d\eta$ with $\eta = (E - E_c)/kT$ and $\eta^* = (E_F - E_c)/kT$. Substituting these into Eq. (1) yields

$$\sigma_{\mathrm{IIS}}(T, \eta^*, p) = (e^2/3h)(2m^* kT/\hbar^2)^{1/2}[n_a/N_i F_p(\eta^*)] \times \int_0^{\infty} \frac{\eta^{p+3/2} f(1 - f)\, d\eta}{\sum_l (l + 1)\sin^2(\delta_l - \delta_{l+1})}, \tag{2}$$

where the scattering integral in Eq. (2) would need to be evaluated numerically when the phase shifts $\delta_l(E)$ are known. For insulating hosts with no compensation at very low T [$kT < 10^{-4}E_G$, with E_G the host band gap] $n_a = N_i$, while for small compensation K ($K \ll 1$) $N_i = n_a + 2KN_D$ for the n-type cases. The dependence of n_a on $E_F - E_c$ will be considered below. In the highly degenerate case $f(1 - f)$ is sharply peaked about E_F and the phase shifts are the values at E_F and change slowly with $E_F(n)$ for $\eta^* \gg 1$. This allows $\lambda_{i,h}[E_F(n)] = \sum_l (l + 1)\sin^2(\delta_l - \delta_{l+1})$ to be removed from the integral. Integrating by parts $\int \eta^{p+3/2} f(1 - f)\, d\eta = (p + 3/2)F_{p+1/2}(\eta^*)$ and σ_{IIS} becomes

$$\sigma_{\mathrm{IIS}}(T, \eta^*, p) = (p + 3/2)[e^2/3h\lambda_{i,h}(n)] \times (2m^*kT/\hbar^2)^{1/2}[F_{p+1/2}(\eta^*)/F_p(\eta^*)]. \quad (3)$$

Evaluating the Fermi integrals for $\eta^* \gg 1$ the leading terms yield for the ratio $[(p + 1)/(p + 3/2)]\eta^{*1/2}$ producing the final result

$$\sigma_{\mathrm{IIS}}(\eta^* \gg 1, p) = (p + 1)[e^2/3h\lambda_{i,h}(n)] \times [2m^*(E_F - E_c)/\hbar^2]^{1/2}. \quad (4)$$

There is a close analogy between standard alloy theory [24,25] and Eqs. (2) and (4). In dilute alloys the residual resistivity $\rho_i = m^*/ne^2\tau_i(E_F)$ where $1/\tau_i = N_i v\langle\sigma_i\rangle$ and using the standard expression for $\langle\sigma_i\rangle$ one finds $\rho_i = (2h/e^2)(N_i/n)(\lambda_{i,h}/k_F)$. The total conductivity for the MIT case is $\sigma = \rho_h^{-1} + \rho_i^{-1}$ where $\rho_h(T \to 0) \to \infty$ [note that the σ contributions are additive, whereas for the alloy $\rho = \rho_h + \rho_i$]. For the dilute alloy $N_i \ll n$ and k_F is determined by the free carrier density n and is virtually constant. For the MIT case with weak compensation $n = n_a \sim N_i$ and $k_F \propto (E_F - E_c)^{1/2}$ and $k_F \to 0$ as $n \to n_{c+}$. The remarkable result for the MIT case for strong enough degeneracy is that $\sigma_i = \rho_i^{-1}$ is independent of the density of itinerant electrons n_a above E_c and depends only on the energy dependence of $\tau_i(E_F) \propto (E_F - E_c)^{1/2}$ and $\lambda_{i,h}(n)$.

Equation (4) can be written as $\sigma_{\mathrm{IIS}} \propto (e^2/h\lambda_{i,h})k_F$ where $k_F = [2m^*(E_F - E_c)/\hbar^2]^{1/2}$. It should be stressed that the use of the expression $\tau = m^*k/2hN_i\lambda_{i,h}$ is crucial in obtaining $\sigma_{\mathrm{IIS}} \propto (e^2/h)k_F$. One cannot obtain this result using either the Conwell-Weisskopf τ_{CW} or the Brooks-Herring τ_{BH}. This form differs from Mott's [26] minimum metallic conductivity $\sigma_M \propto (e^2/h)k_F^2 l$ because it lacks the extra $k_F l$ factor and because k_F depends only on the itinerant electrons above E_c while Mott's k_F depended on the total doping density N_d. Significantly, the result in (4) is independent of the correlation length $[\xi(E)/\xi_0 = [(E - E_c)/E_0]^{-\nu}]$ exponent ν. If $\xi(E)$ is inserted into (4), one finds $\sigma_{\mathrm{IIS}} \propto (2m^*E_0/\hbar^2)^{1/2}(\xi_0/\xi)^{1/2\nu}$. For $\nu = 1$ $\sigma_{\mathrm{IIS}} \propto \xi^{-1/2}$, similar to a result obtained by Kaveh and Mott [14]. Their result was obtained with localization and interaction corrections and depended on the relative magnitude of the Hartree and exchange contributions. The present result coming from incoherent IIS can be written as $\sigma_{\mathrm{IIS}} \sim e^2/\hbar\lambda_{\mathrm{dB}}$, where $\lambda_{\mathrm{dB}} = h/p_F = h/[2m^*(E_F - E_c)]^{1/2}$ is the de Broglie wavelength. In the critical regime $n/n_c - 1 \ll 1$ $\lambda_{\mathrm{dB}} < \xi(n)$, the dominant scattering is incoherent, which is why σ_{IIS} is independent of ν. Electron-electron interactions through screening can affect the phase shifts, but the phase shifts only enter the prefactor σ_0 for $\eta^* \gg 1$. Using $(E_F - E_c)/E_0 = (n/n_c - 1)^{\beta}$ one obtains $\sigma_{\mathrm{IIS}} \propto (n/n_c - 1)^{\beta/2}$, which yields the result $s = \frac{1}{2}$ for $\beta = 1$, which is the accepted value of β. Since $E_F - E_c = E_0$ at $n = 2n_c$ the quantity $(2m^*E_0/\hbar^2)^{1/2} = k_F(2n_c) = (3\pi^2 2n_c/v)^{1/3}$ where v is the number of valleys in the n-type many-valley semiconductor. For p-type cases v is the orbital degeneracy of the Γ_8 states at the top of the valence band neglecting the spin-orbit split off Γ_7 states. For n-type cases the large valley orbit splittings remove the degeneracy of the donor levels. The impurity bands for Si consist of 1s-A_1, 1s-T_2, and 1s-E bands which strongly overlap for $n > n_c$. Assuming all of these band states exist below E_{CB} then v remains unchanged. The conductivity prefactor $\sigma_0(n_c, p, \lambda_{i,h})$ is now determined if the phase shifts and $\lambda_{i,h}$ are known. Conversely, the experimental σ_0 can be used to determine values of $\lambda_{i,h}$ for a given p since the n_c are known. For screened Coulomb potentials the phase shifts can be calculated subject to the Friedel sum rule and calculated values of $\lambda_{i,h}$ can be compared with the experimental values.

Table I gives the experimental values of n_c and σ_0 and calculated values of $(e^2/3h)k_F(2n_c)$. The $\lambda_{i,h}$ $\{\lambda_{i,h} = (e^2/3h)[k_F(2n_c)/\sigma_0]\}$ given are for the v values in Table I. If one used $p = \frac{1}{2}$ corresponding to $\sigma_B = n_a e^2\tau(E_F)/m^*$ the $\lambda_{i,h}$'s would increase by 50%. The quantity $\lambda = 1$ for a single phase shift $\delta_0 = \pi/2$. For two phase shifts δ_0, $\delta_1 = \delta_0/m$, $\lambda = 0.39$ for $m = 3$ and 0.78 for $m = 9$. For three phase shifts $\delta_2 = \delta_1/q$ the λ are reduced further as shown in Table I. Seeger [27] has reported phase shifts for a screened Coulomb potential ($Z = 1$) corresponding to $m = 4.6$, $q = 5.7$, and $\lambda = 0.41$. The experimental values of $\lambda_{i,h}$ fall into two groups, one clustering around 0.17 for Si:P, Si:As, and Ge:Sb, and a second with $0.36 < \lambda_{i,h} < 0.57$. One expects a difference for n- and p-type cases because of the different character $(s, p, \ldots)$ of the wave functions near the conduction band and valence band edges. The donor differences for the same host between Si:Sb, Si:P, and Si:As and between Ge:As and Ge:Sb (the values of σ_0 are less accurate for Si:Sb and Ge:As) probably reflect the effect of the strong short range central cell potential (unscreened by carriers) on the phase shifts and $\lambda_{i,h}$. The central cell potential leads to donor binding energy differences (dilute limit) $E_D - E_{\mathrm{eff.mass}}$ that are understood. The $\lambda_{i,h}$ do not show impurity variations simply related to $E_D - E_{\mathrm{eff.mass}}$. Comparison of the Yamanouchi *et al.* [28] Si:P data with Eq. (4) shows

TABLE I. Conductivity prefactors and phase shift sums. In the first column, the value of v is given in parentheses.

	$n_c \times 10^{-18}$ (cm^{-3})	σ_0 (S/cm)	$(e^2/3h)k_F(2n_c)$ (S/cm)	$\lambda_{i,h}$ ($p = 0$)	Theory
Si:P (6)	3.73	260	42.9	0.17	$2\delta_l, \delta_1 = \delta_0/m$
Si:As (6)	8.57	376	56.6	0.15	$m = 3, \lambda = 0.39$
Si:Sb (6)	2.92	110	39.5	0.36	$m = 9, \lambda = 0.78$
Si:B (2)	4.06	152	63.6	0.42	$3\delta_l, \delta_1 = \delta_0/m, \delta_2 = \delta_1/q$
Ge:As (4)	0.34	56	22.1	0.39	$m = 3, q = 6, \lambda = 0.27$
Ge:Sb (4)	0.155	92	17.0	0.18	$m = 9, q = 6, \lambda = 0.71$
Ge:Ga (2)	0.186	40	22.8	0.57	$m = 4.6, q = 5.7, \lambda = 0.41$ [27]

$\lambda_{i,h}(n)$ changes by about 15% between n_c and $2n_c$ and less than 45% over a factor 25 in n, thus clarifying the reason for the large width of the scaling regime for $s \sim \frac{1}{2}$. How large must $\eta^* = E_F - E_c/kT$ be to ensure $s \sim 0.5$? The slope of $F_{1/2}(\eta^*)/F_0(\eta^*)$ versus η^* is 0.461, 0.475, 0.483, 0.487, and 0.490 at η^* equal to 8, 10, 12, 14, and 16, respectively. Numerical integration of the scattering integral in Eq. (3) confirms the change in $\lambda_{i,h}$ with η^* is small for $\eta^* > 5$, justifying the removal of the phase shift sum from the integral in Eq. (3). Despite uncertainties, the results in Table I demonstrate IIS can account for the magnitude of σ_0.

Traditionally, the prefactor σ_0 has been given as $A\sigma_M$ where σ_M is the Mott minimum metallic conductivity [Si:P $\sigma_M = 20$ S/cm, $A = 13$]. Using localization and interaction corrections to explain the scaling of $\sigma(n, T = 0)$ Bhatt and Ramakrishnan [29] suggest $\sigma_0 \sim \sigma_B(n = n_c)$ and find $A \sim 12$ for Si:P. This calculation and theoretical efforts for two decades presumed $\sigma_B(n, T = 0)$ could not explain the scaling. With σ_B accounting for the scaling the logical prefactor is $\sigma_0 = \sigma_B(2n_c) \propto [e^2(2n_c)^{1/3}/h\lambda_{i,h}]$ which is always larger than σ_M. A detailed comparison of the experimental σ_0's with theory requires accurate values of δ_l.

Although the scaling and the exponent $s = \frac{1}{2}$ [for $\beta = 1$] are independent of the form of the DOS just above E_c other physical quantities might depend on the DOS and p. These include the density of itinerant electrons n_a above E_c, the mobility μ ($\mu = \mu_H = \mu_{\mathrm{drift}}$ for $\eta^* \gg 1$), the charge diffusion coefficient $D \propto (E_F - E_c)\mu/e$ (for $\eta^* \gg 1$), the mean-free-path l, and the important parameter $k_F l$. The scaling of the Hall coefficient [$1/R_H(n, T \to 0) \propto (n/n_c - 1)^g$, $0.34 < g < 0.44$, for Si:P, Si:As, Si:B [8]] has been interpreted [15] as determining the itinerant carrier density $n_a = \gamma n_c(n/n_c - 1)^g$. Based on $N(E) = N(E_c) + C(n)[(E - E_c)/E_0]^p$ one calculates $n_a(T = 0)$ to be for $\eta^* \gg 1$

$$n_a(T \to 0) = N(E_c)[E_F - E_c(n)] + [C(n)E_0/(p + 1)] \times \{[E_F - E_c(n)]/E_0\}^{p+1}, \quad (5)$$

where the relative importance of the two terms is not known. It might appear that the first term in (5) would lead to an exponent $g \sim 1$. That need not be the case and it must be emphasized $E_c(n)$ will have to decrease for a rigid $N(E)$ since $n_l(T \to 0) = \int_{E_d}^{E_c(n)} N(E)\,dE$ must decrease with increasing n. This suggests $E_c(n)$ decreases with n and if $N[E_c(n)]$ decreases as $E_c(n)$ decreases, consistent with $E_F - E_c = E_0(n/n_c - 1)$ it is possible to obtain $g < 1$. This could also happen if $C(n)$ were negative. If the first term in Eq. (5) is dominant, then the role of the exponent p in determining the scale of n_a is unclear. The scaling of n_a will be discussed in detail elsewhere. Based on the Cohen *et al.* [30] physical notion the mobility [$\mu = e\tau/m^* = ek_F/2h\lambda_{i,h}N_i \propto (n/n_c - 1)^{1/2-g}$] must not diverge as $n \to n_c$, one requires $g < \frac{1}{2}$ [in general $g < s$], which is consistent with the known Hall data. D scales with the same exponent as $k_F l$ which is slightly larger than 1, namely $1 + s - g$. A previous analysis [15] using the excess scaling CESR linewidth data [31] yielded $1/\tau_c \propto D \propto (n/n_c - 1)^\eta$ with $\eta = 0.95$ for Si:As and 0.90 for Si:P. To satisfy the Einstein relation this required $\beta = 0.76$ for Si:As and 0.73 for Si:P. That analysis was based on l varying slowly near n_c so that $1/\tau_c$ and D scaled with the same exponent. The present analysis suggests $l \to 0$ as $n \to n_c$ with a scaling exponent $1 - g$. The previous analysis employed $k_F \propto (n_a)^{1/3} \propto (n/n_c - 1)^{g/3}$ and required the effective mass to scale with an exponent $2g/3 - \beta$. For the present case $m^* = \text{const}$ since the theory is a one electron theory neglecting e-e interactions except through the screening in the phase shifts. If one uses the scaling $1/\tau_c$ from the CESR results and $k_F l = 2(E_F - E_c)\tau_c/\hbar$ the scaling exponent for $k_F l$ is 0.05 for Si:As and 0.1 for Si:P, thus leading to a very small change in $k_F l$ between $2n_c$ and $1.01n_c$. The CESR is done in the absence of an applied dc voltage and the magnitude of the cross section might differ for this case, but the scaling with $n/n_c - 1$ should have been the same. This difference is not understood. The lack of a theoretical understanding of the exponent g has no effect on the scaling result in Eq. (4) and the basic result $s = \frac{1}{2}$ when $\beta = 1$.

Mott's σ_M derivation was based on the Ioffe-Regel criterion that $k_F l \geq 1$ and the notion that $n_a = n \sim N_d$. The present analysis demonstrates $k_F l \propto (E_F - E_c)^{3/2}/N_i$. The scaling of N_i ($N_i \sim n_a$) is much slower than $(E_F - E_c)^{3/2}$ leading to the scaling of $k_F l$. To keep $k_F l$ from scaling would also argue no scaling of D and would

require $g = 3/2$ and would produce a divergence of μ. Both of these consequences appear untenable and argue the importance of $g < s$.

The role of neutral impurity scattering (NIS) needs to be considered, because as $n \to n_{c+}$ the density of neutral impurities N_n approaches the doping density $n = N_D - N_A \sim N_D$. For $1/\tau_n = N_n v \langle \sigma_n \rangle$ and assuming the two scattering rates are additive (the only plausible assumption) one has $\tau_{\text{eff}}^{-1} = \tau_i^{-1} + \tau_n^{-1} = (4\pi v/k^2)[N_i \lambda_{i,h} + N_n \lambda_{n,h}]$ where $\lambda_{n,h}$ is the same form as $\lambda_{i,h}$, but the phase shifts for neutral impurity scattering must satisfy the restriction $\Sigma_l (2l + 1)\delta_l = 0$. This leads to a correction factor for σ_{IIS} of the form $[1 + (N_n/N_i)(\lambda_{n,h}/\lambda_{i,h})]^{-1}$. Since $\lambda_{n,h} \ll \lambda_{i,h}$ the correction is only of possible importance close to n_c where the ratio N_n/N_i becomes large. This ratio can be estimated from the Hall data using $n_a = \gamma n_c (n/n_c - 1)^g$, $n_a = N_i$, $N_n + N_i = n$. The ratio N_n/N_i for Si:P ($\gamma = 1.9$, $g \sim 0.34$) is 0.24 at $1.1 n_c$, 1.5 at $1.01 n_c$, and 4.3 at $1.001 n_c$. $\lambda_{n,h}/\lambda_{i,h}$ is not known for these systems, but for impurities in alkali metals has been calculated by Ball *et al.* [32] to be of order 0.05 for Li:Ag/Li:Mg. Kohn and Vosko [33] have obtained a ratio 0.14 for Cu:Ag/Cu:Zn. For systems like Si:P, Ge:As, and Ge:Ga the potentials of the impurity and host atoms are similar and the phase shifts contributing to $\lambda_{n,h}$ may be much smaller than for Li:Ag and Cu:Ag. Two other reasons why NIS may be even less important than the above expression would indicate are (1) the increasing importance of spatial inhomogeneity and of "percolating" conducting filaments [16] as $n \to n_c$; (2) in the regime $k_F l < 1$ the electron wavelength is much greater than the neutral donor spacing and scattering from individual neutral donors becomes problematic. This is also the regime where weak localization corrections badly break down and the Heisenberg uncertainty principle says the itinerant electron's position is not determined to better than $2\pi/k_F$, which becomes larger than the donor spacing. The crucial $\sigma(n, T \to 0)$ data for Si:P and Ge:Ga exhibit scaling consistent with $\sigma_{\text{IIS}} \propto (E_F - E_c)^{1/2}$ for $n/n_c - 1 < 0.001$ with no observable deviations, or far into the regime where $k_F l < 1$. This suggests NIS is not important, but also argues the Ioffe-Regel criterion is not applicable for these systems.

In summary, it is shown the Boltzmann conductivity can explain the $T = 0$ scaling of the conductivity. In the degenerate regime for the weakly compensated case, employing the two-component model and a mobility edge from Anderson localization, the Boltzmann conductivity for ionized impurity scattering explains the scaling exponent $s = \frac{1}{2}$ first observed for Si:P and the large width of the scaling regime. The scaling of the diffusion coefficient, Hall coefficient, and the mobility scaling can also be explained, but the role of DOS on the critical behavior remains unclear. The scaling exponent s doesn't depend on ν or the form of the DOS.

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