

Nonrandom doping and elastic scattering of carriers in semiconductors

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High-density delta doping of semiconductors may result in partial ordering of dopant atoms. Under suitable circumstances, periodic delta doping leads to significant suppression of elastic scattering and a consequent enhancement in charge carrier mobility.

The mobility of carriers in doped semiconductors is to a large measure determined by the elastic scattering of these carriers from the dopant ions, i.e., by the interaction potential

$$V(\mathbf{r}) = \sum_i v(\mathbf{r} - \mathbf{R}_i). \quad (1)$$

Here \mathbf{R}_i represents the ion positions and

$$v(\mathbf{r}) = \int \frac{d^3\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{4\pi e^2}{q^2 \epsilon(\mathbf{q})} \quad (2)$$

is the Coulomb potential of a bare ion statically screened by the dielectric constant $\epsilon(\mathbf{q})$, where \mathbf{q} is the scattered wave vector.

Suppose that we are interested in a particle with initial wave vector \mathbf{k} , energy $E_i(\mathbf{k})$, and velocity v_k . Operationally it has a scattering rate τ_{ei}^{-1} from the donor ions and a mean free path $l_k = v_k \tau_{ei}$. If $kl_k \gg 1$, we may reliably calculate the elastic ionized impurity scattering rate τ_{ei}^{-1} to lowest order in the impurity potential. Using the first term in the Born series, we obtain (Fermi's golden rule)

$$\tau_{ei}^{-1} = \frac{2\pi}{\hbar} \int \frac{d^3\mathbf{q}}{(2\pi)^3} |V(\mathbf{q})|^2 \delta[E(\mathbf{k}) - E(\mathbf{k} - \mathbf{q})] \quad (3)$$

for the transition rate. Here $V(\mathbf{q})$ is the Fourier transform of $V(\mathbf{r})$,

$$V(\mathbf{q}) = \sum_i \int d\mathbf{r} v(\mathbf{r} - \mathbf{R}_i) e^{-i\mathbf{q}\cdot(\mathbf{r} - \mathbf{R}_i)} e^{-i\mathbf{q}\cdot\mathbf{R}_i}. \quad (4)$$

It follows that

$$|V(\mathbf{q})|^2 = s(\mathbf{q}) |v(\mathbf{q})|^2, \quad (5)$$

where $s(\mathbf{q})$ is the structure factor

$$s(\mathbf{q}) = \left| \sum_i e^{i\mathbf{q}\cdot\mathbf{R}_i} \right|^2 \quad (6)$$

and

$$v(\mathbf{q}) = 4\pi e^2 / q^2 \epsilon(\mathbf{q}). \quad (7)$$

As will be seen later, even in the "random" case a reduction in scattering rate occurs because, for small q

$$s(\mathbf{q}) = n(1 - f), \quad (8)$$

where f is the fraction of occupied sites. The factor $(1 - f)$ appears because impurity atoms sit on discrete lattice sites and double occupancy of a site is not allowed. In the dilute limit, $f \rightarrow 0$ and Eq. (8) gives the result $s(\mathbf{q}) = n$, so that the scattering rate given by Eq. (3) is n times the scattering rate from a single dopant ion.¹

In this letter we analyze $s(\mathbf{q})$ for dopant atoms placed on an underlying three-dimensional lattice. We then numerical-

ly evaluate a simple model of correlated impurity doping and show that it leads to a decrease in the structure factor $s(\mathbf{q})$ at small q and a corresponding decrease in elastic ionized impurity scattering rate, τ_{ei}^{-1} .

Layer-by-layer crystal growth of GaAs using methods such as molecular beam epitaxy is possible because Ga atoms are able to diffuse on the exposed GaAs surface before final bonding to a crystal lattice site. A recent development of this monolayer deposition technique is delta doping,² where the Ga flux is interrupted and a fraction of a monolayer of impurity atoms such as Be with sheet concentration n_s is deposited on the GaAs surface. Typically, n_s is in the range 10^{10} cm^{-2} to greater than $1.3 \times 10^{14} \text{ cm}^{-2}$ so that the fraction of electrically active occupied sites, f , can be greater than 0.2.³

We consider the case where possible dopant atom positions are specified by the vector, $\mathbf{r}_{LMN} = a\mathbf{L} + b\mathbf{M} + c\mathbf{N}$, where L , M , and N are integers (see Fig. 1), c is in the z direction, and a and b form a square lattice in the x - y plane. For (001) oriented GaAs $|a| = |b| = 3.99 \text{ \AA}$ and $|c| = 5.65 \text{ \AA}$. The integer l is fixed by the spacing ΔZ between planes containing dopant atoms. The reciprocal lattice vectors of this Ga lattice \mathbf{r}_{LMN} are denoted by \mathbf{Q}_n . Taking Eq. (6) we obtain an ensemble average structure factor for n dopant atoms given by

$$s(\mathbf{q}) = fn \sum_{L,M,N} C_{LMN} e^{i\mathbf{q}\cdot\mathbf{r}_{LMN}}, \quad (9)$$

where $f^2 C_{LMN} = \langle \epsilon_{LMN} \epsilon_{000} \rangle$. The quantity

$$\epsilon_{LMN} = \begin{cases} 1 & \text{site } LMN \text{ occupied} \\ 0 & \text{site } LMN \text{ unoccupied} \end{cases}$$

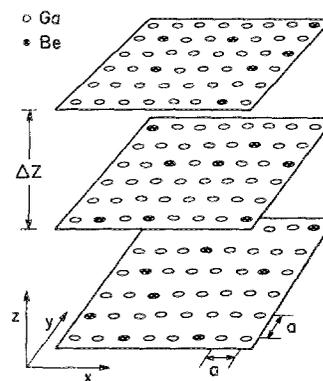


FIG. 1. Schematic diagram of Be delta-doped sheets in (001) oriented GaAs. For GaAs $a = 3.99 \text{ \AA}$. The numerical example in the text uses $\Delta Z = 39.5 \text{ \AA}$ corresponding to seven Ga bilayer spacings. Note that $\pi/\Delta Z = 7.94 \times 10^9 \text{ cm}^{-1}$.

and $\langle \dots \rangle$ denotes an ensemble average. The known fractional occupation of all Ga sites in a doped plane is $\langle \epsilon_{LMN} \rangle = f$. The correlation coefficients C_{LMN} have values $1/f$, 1 , and 0 for the extreme cases of perfect correlation, completely random correlation, and perfect anticorrelation, respectively. We rewrite Eq. (9) by adding and subtracting 1 from C_{LMN} so that

$$s(\mathbf{q}) = fnB(\mathbf{q} - \mathbf{Q}_n) + fn \sum_{LMN} (C_{LMN} - 1)e^{i\mathbf{q} \cdot \mathbf{r}_{LMN}}, \quad (10)$$

where

$$B(\mathbf{q}) = \sum_{L,M,N} e^{i\mathbf{q} \cdot \mathbf{r}_{LMN}}$$

is the Bragg scattering result from the perfect Ga lattice specified by \mathbf{r}_{LMN} and is nonzero only at reciprocal lattice vectors \mathbf{Q}_n . For low-energy charge carriers with small k such lattice vectors ($\mathbf{Q}_n \neq 0$) are not accessible and this term plays no role in the transport as long as the layer spacing ΔZ is not too large, i.e., $k < \pi/\Delta Z$.

If there is no correlation between dopant atoms in different planes, then $C_{LMN} = 1$ for $N \neq 0$ and

$$s(\mathbf{q}) = fnB(\mathbf{q} - \mathbf{Q}_n) + fn \sum_{LM} (C_{LM} - 1)e^{i\mathbf{q} \cdot \mathbf{r}_{LM}}, \quad (11)$$

where $C_{LM} = C_{LMO}$ and $\mathbf{r}_{LM} = \mathbf{r}_{LMO}$ is in the $x - y$ plane. The structure factor $s(\mathbf{q})$ thus reduces to a form which only involves correlations in the plane.

We now examine two limits of our model: the completely random case and the perfectly ordered in-plane case. We denote by P the quantity in Eq. (11):

$$P = f \sum_{LM} (C_{LM} - 1)e^{i\mathbf{q} \cdot \mathbf{r}_{LM}}. \quad (12)$$

In the completely random case all $C_{LM} = 1$ except $C_{00} = 1/f$, since a site's occupancy is always correlated with itself. Thus,

$$s(\mathbf{q}) = fnB(\mathbf{q} - \mathbf{Q}_n) + (1 - f)n. \quad (13)$$

The first term is the imprint of the underlying lattice leading to Bragg spots with intensity n^2 . The second term in Eq. (13) represents elastic scattering which is generally nonzero for *any* wave vector \mathbf{q} . The factor $(1 - f)$ is a direct result of excluding double occupancy of a site and is the correlation effect referred to earlier which gives rise to Eq. (8).

We now consider the case of perfect in-plane ordering of dopant atoms⁴ whose positions form a two-dimensional superlattice with reciprocal lattice vectors \mathbf{q}_p . In this situation $C_{LM} = 1/f$ for those L, M corresponding to the two-dimensional superlattice position separations and $C_{LM} = 0$ otherwise. Therefore $P = 0$ unless \mathbf{q} has a projection into the $x - y$ plane that is a two-dimensional reciprocal lattice vector \mathbf{q}_p . The resulting Bragg rods pass through the \mathbf{q}_p as shown in Fig. 2(c). Using Eq. (11) it is possible to show that those Bragg rods which contain a reciprocal lattice vector of the underlying two-dimensional Ga lattice are missing. Scattering *near* $\mathbf{q} = 0$ is completely suppressed. The "scattering" at exactly $\mathbf{q} = 0$ is irrelevant and does not contribute in the present context. In most cases of interest charge carriers

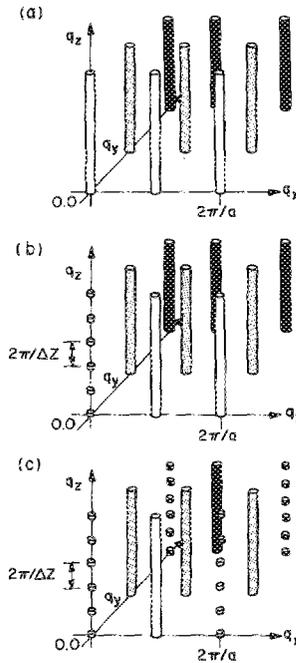


FIG. 2. (a) Schematic diagram of Bragg diffraction rods for a single plane of dopant atoms in a superlattice. (b) Bragg diffraction rods and spots for planes similar to (a) but separated by ΔZ and no correlations between dopants in different planes. (c) Same as (b) except potential dopant sites are required to be on the lattice defined by \mathbf{r}_{LMN} .

have wave vector $k < q_p/2$, implying a zero elastic scattering rate.

For a more realistic situation where there are intermediate correlations we would expect a modification of the scattering rate. In reality correlations depend on details of crystal growth and doping processes. The rate of deposition of dopant atoms, the temperature of substrate, etc., all play a role. It is not the purpose of this letter to investigate in any detail such processes. Rather, we show numerically that even a modest correlation effect can lead to a significant suppression of the elastic scattering rate at high dopant levels.

Since a dopant atom such as Be has a different electronic structure and radius than the substitutional atom (e.g., Ga in GaAs) it is plausible that there is a short-range potential between two such dopants. When placed on a GaAs growth surface a Be atom will diffuse by hopping from Ga site to Ga site. A repulsive potential will bias the hops so as to partially eliminate, for example, near neighbor occupations. In this picture the Be atoms will anneal towards a periodic lattice.

As a numerical example, we simulated placing Be atoms on a square lattice with 1000×1000 sites using periodic boundary conditions. Atoms of Be are placed on Ga sites one at a time according to the following procedure. A site is chosen randomly. That site becomes occupied unless it is already occupied or has one or more nearest neighbors. The process is iterated until a number of sites are occupied, 2×10^5 sites in our example corresponding to $f = 0.2$. From the resulting configurations, the C_{LM} are calculated. As expected for a random correlation large L or large M gives $C_{LM} \approx 1$. Using only statistically significant C_{LM} (i.e., $|C_{LM} - 1| > 1/\sqrt{2} \times 10^5$ and $|L| < 6$ and $|M| < 6$), the

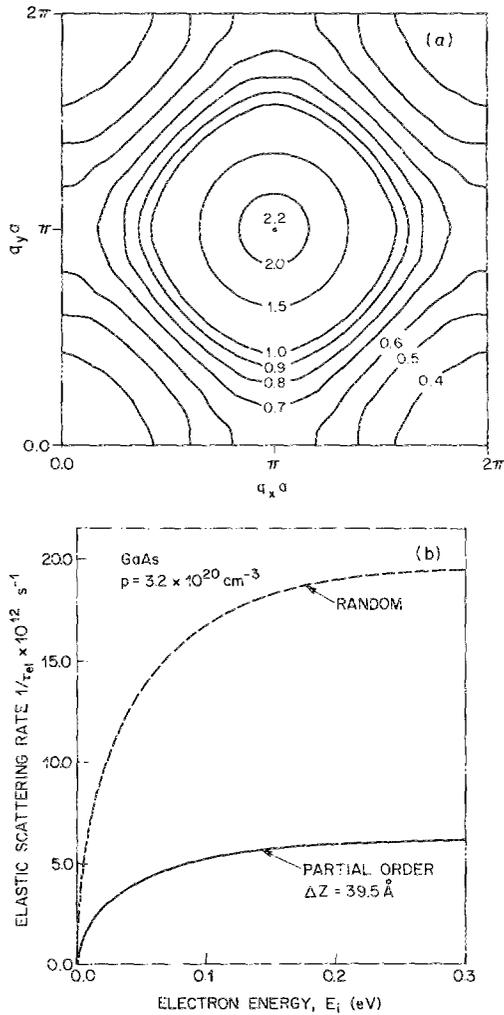


FIG. 3. (a) Contour plot of P/P_R for the numerical example described in the text where P_R is the random value of P . In this case $f = 0.2$ and there is zero nearest neighbor occupancy. In GaAs $\pi/a = 7.86 \times 10^7 \text{ cm}^{-1}$. (b) Total elastic electron scattering rate τ_{el}^{-1} from ionized impurities for the random and partially ordered case as a function of conduction-band electron energy E_i in p -type GaAs with $n^{p \text{ type}} = p = 3.2 \times 10^{20} \text{ cm}^{-3}$. The parameters used in the calculations were the same as used in Ref. 5. Note, for $E_i = 0.3 \text{ eV}$ $k = 7.42 \times 10^6 \text{ cm}^{-1} < \pi/\Delta Z < \pi/a$.

quantity $P(q_x, q_y)$ was calculated and the result is shown as the contour plot in Fig. 3(a). Near $\mathbf{q} = 0$ P is reduced from its random value by a factor of less than 0.4.

Using Eq. (3) and the appropriate $\epsilon(\mathbf{q})$ for holes as

discussed in Ref. 5 we have calculated τ_{el}^{-1} as a function of initial energy E_i for minority carriers injected into p -type GaAs. The results are plotted in Fig. 3(b). The broken curve is for a randomly doped three-dimensional sample with average impurity concentration $n^{p \text{ type}} = 3.2 \times 10^{20} \text{ cm}^{-3}$ using $s(\mathbf{q}) = n^{p \text{ type}}$. The solid curve for τ_{el}^{-1} is found in the same way except using $s(\mathbf{q})$ from the numerical result described above and $\Delta Z = 39.5 \text{ \AA}$ chosen so that the average bulk impurity concentration, $n^{p \text{ type}} = 3.2 \times 10^{20} \text{ cm}^{-3}$, is the same as the random case. As may be seen, the reduction in τ_{el}^{-1} for the partially ordered delta-doped sheets is greater than a factor of 3.

In summary, because impurities occupy semiconductor crystal lattice sites there is a reduction $(1 - f)$ in small wave-vector elastic ionized impurity scattering. Additional ordering effects⁴ and high-density delta doping of semiconductors may result in a further reduction in elastic ionized impurity scattering. In particular a reduced τ_{el}^{-1} could significantly improve the performance of high-speed heterojunction bipolar transistors which utilize a thin, very heavily doped p -type base.^{6,7}

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¹ $S(\mathbf{q}) = n$ is the often quoted result used for calculating elastic ionized impurity scattering rates from a random set of impurities. This situation was first analyzed by W. Kohn and J. M. Luttinger, Phys. Rev. **108**, 590 (1957); also, see for example, P. Chattopadhyay and H. J. Queisser, Rev. Mod. Phys. **53**, 745 (1981).

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³A room temperature mobility $\mu = 38 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ has been measured in delta-doped (001) oriented GaAs with an electrically active Be sheet carrier concentration $n_c^{p \text{ type}} = 1.3 \times 10^{14} \text{ cm}^{-2}$, J. E. Cunningham (private communication).

⁴Experimental evidence for in-plane ordering of dopant atoms in semiconductors is beginning to emerge. K. Akimoto, J. Mizuki, I. Hirose, T. Tatsumi, H. Hirayama, N. Aizaki, and J. Matsui, Extended Abstracts 19th Conf. Solid State Devices & Materials, Busines Center for Academic Societies, Japan, Tokyo, 1987, pp. 463-466; L. C. Feldman, R. L. L. Hedrick, and I. K. Robinson (unpublished) have shown that one-third of a monolayer ($f = 0.33$) of ordered B can be preserved at the interface between an overgrown Si layer and a Si(111) substrate.

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⁶A. F. J. Levi, Electron. Lett. **24**, 1273 (1988).

⁷R. N. Nottenburg, Y. K. Chen, and M. B. Panish (unpublished).