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Field Inhomogeneity in Electroreflectance*

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A criterion for the validity of the uniform-field approximation in electroreflectance experiments is derived and discussed. It is shown that a proper choice of impurity concentration can minimize the inhomogeneity for a given magnitude of the electric field. Using germanium as an example, the optimum doping levels are given for various values of the electric field. These optimal impurity concentrations minimize the mixing of the real and imaginary parts of the change in the dielectric function with electric field, so that the observed line shapes can be easily interpreted. The results show that the uniform-field approximation can be used with electric fields as high as 10^5 V/cm, provided the proper doping levels are used.

I. INTRODUCTION

THERE has been much discussion in the literature concerning the correct interpretation of the line shapes observed in electroreflectance (ER) by Aspnes and Frova[1] and others.[2–4] Since the electric field in the space-charge region of a semiconductor surface varies with the distance from the surface, so does the dielectric function. The reflection of light from a surface region where the dielectric function varies with distance has been discussed by Aspnes and Frova.[1]

The results[1–4] show that for near-intrinsic Ge at certain wavelengths and fields, the dielectric function may vary rapidly enough over the penetration depth of the light to cause the change in reflectance due to the application of an electric field to be significantly different from that due to a uniform field. However, in this paper we will show that for the magnitude of the electric fields used, there are samples with certain impurity concentrations or doping levels which will give line-shape results very close to the uniform-field approximation. It will be shown that for each value of the electric field there is an ideal doping level. The results will be presented in terms of a product of the fractional change in the electric field over an effective penetration depth times a factor determined by the electric field dependence of $\Delta\epsilon$. Experimental line shapes as well as the one-electron line shapes[1–4] will be discussed.

II. DISCUSSION

Aspnes and Frova[1] have recently shown that in a modulated reflectance experiment, mixing of the real and imaginary parts of the modulated dielectric constant can occur due to a nonuniform perturbation over the penetration depth of the light. In particular, the measured $\Delta\epsilon$ denoted by $\langle\Delta\epsilon\rangle$ is given by

$$\langle\Delta\epsilon\rangle=\langle\Delta\epsilon_1\rangle+i\langle\Delta\epsilon_2\rangle=-2iKe^{2iKz_s}\times\int_{-\infty}^{z_s}e^{-2iKz'}\Delta\epsilon(z')dz', \quad (1)$$

where $K=2\pi(n+ik)/\lambda$, z_s is the surface coordinate, and $\Delta\epsilon(z)=\Delta\epsilon(\mathcal{E}(z))$ is the spatially dependent change in the dielectric constant with field. Aspnes and Frova mention that a field inhomogeneity can strongly modify the ER line shape even when the uniform-field approximation would appear to be valid. We would like to clarify this remark and point out the conditions for validity of the uniform-field approximation.

In reality what one wants is a "uniform perturbation" of the dielectric constant over the penetration depth of the light. Because ϵ may vary more rapidly as a function of distance from the surface than does the electric field $\mathcal{E}$, an approximate uniform field does not always imply an equally good approximate uniform perturbation. To obtain a relation between the two, consider Eq. (1). Expanding $\Delta\epsilon(z')$ in a Taylor series about z_s, we have

$$\langle\Delta\epsilon\rangle=-2iK\sum_{m=0}^{\infty}\frac{\Delta\epsilon^{(m)}(z_s)}{m!}\int_{-\infty}^{0}y^m e^{-2iKy}\,dy, \quad (2)$$

where $y=z'-z_s$ and $\Delta\epsilon^{(m)}=[d^m(\Delta\epsilon)/dz^m]z_s$. Upon integration we have

$$\langle\Delta\epsilon\rangle=\Delta\epsilon(z_s)\left(1+\sum_{m=1}^{\infty}\frac{\Delta\epsilon^{(m)}(z_s)}{\Delta\epsilon(z_s)}\frac{1}{(2iK)^m}\right). \quad (3)$$

If the perturbation is uniform, all derivatives of $\Delta\epsilon$ vanish and $\langle\Delta\epsilon\rangle\rightarrow\Delta\epsilon(z_s)$. The uniform-perturbation approximation requires that the sum in large parentheses be small compared to 1. To show that we may approximate this sum by the first term, consider the following example. Let $\Delta\epsilon(z)\propto e^{az}$, where a may be complex. Then $\Delta\epsilon^{(m)}(z_s)/\Delta\epsilon(z_s)=a^m$ and

$$\langle\Delta\epsilon\rangle=\Delta\epsilon(z_s)\left[1+\sum_{m=1}^{\infty}\left(\frac{a}{2iK}\right)^m\right]. \quad (4)$$

If $|a|\ll|2iK|=[(4\pi n/\lambda)^2+\alpha^2]^{1/2}$, where α is the ab-

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[1] D. E. Aspnes and A. Frova, Solid State Commun. 7, 155 (1969).

[2] F. Evangelisti and A. Frova, Solid State Commun. 6, 621 (1968).

[3] B. O. Seraphin and N. Bottka, Solid State Commun. 7, 497 (1969).

[4] A. Frova and D. E. Aspnes, Phys. Rev. 182, 795 (1969).

sorption coefficient, we can neglect the terms for $m>1$. Physically this means that the wavelength λ/n or the penetration depth $1/\alpha$ of the light must be small compared to the distance in which the perturbation changes significantly, which is given by $1/|a|$. We thus have the result that even if the light penetrates to large depths, when α is small, variations in $\Delta\epsilon$ will be averaged out by the rapidly oscillating factor $e^{-i4\pi nz'/\lambda}$ in Eq. (1) provided $\lambda/n \ll 1/|a|$.

For perturbations of the type such as given in the above example, only the first term in the sum of Eq. (3) will be important. In order to obtain the uniform-perturbation approximation this first term should be small compared to unity. Thus, if the quantity

$$\frac{1}{|2K|}\left|\frac{d(\Delta\epsilon)/dz}{\Delta\epsilon(z)}\right|_{z_s} \ll 1, \tag{5}$$

the ER signal can be treated as coming from a uniform perturbation, which is identical with the criterion given by Aspnes and Frova.[1] This is just the fractional change in $\Delta\epsilon$ over the distance $1/|2K|$. The same result is obtained by keeping only the first-order term in the Taylor-series expansion of $\Delta\epsilon(z')$ in Eq. (2).

Equation (5) may be written

$$\frac{1}{|2K|}\left|\frac{d\ln\mathcal{E}}{dz}\right|_{z_s}\left|\frac{d\ln\Delta\epsilon}{d\ln\mathcal{E}}\right|_{z_s} \ll 1. \tag{6a}$$

That is, the condition for the uniform-perturbation approximation is

$$(1/|2K|)R_1R_2 \ll 1, \tag{6b}$$

where $R_1=|d\ln\mathcal{E}/dz|$ and $R_2=|d\ln\Delta\epsilon/d\ln\mathcal{E}|$. While R_2 depends on $\mathcal{E}$ and $\hbar\omega$ through the functional dependence of $\Delta\epsilon(\mathcal{E},\hbar\omega)$, R_1 depends only on the fractional change of field with distance. From standard texts[5,6] we have that

$$R_1=\frac{1}{L_D}\left|\frac{\sinh u_S-\sinh u_B}{F(u_S,u_B)}\right|, \tag{7}$$

where

$$F(u_S,u_B)=\sqrt{2}[(u_B-u_S)\sinh u_B+\cosh u_S-\cosh u_B]^{1/2},$$

L_D is the intrinsic Debye length, u_S is the surface potential, and u_B is the bulk potential in units of kT/q. Of the three factors in Eq (6), only R_1 can be minimized by adjusting the impurity concentration (u_B) of the sample for a given field. Both K and R_2 are determined by the field and photon energy.

In Fig. 1, $\log R_1$ is plotted versus $\log\mathcal{E}$ for four different sample dopings. For the $u_B=6$ sample, we have plotted $\log R_1$ for both the accumulation and depletion space-

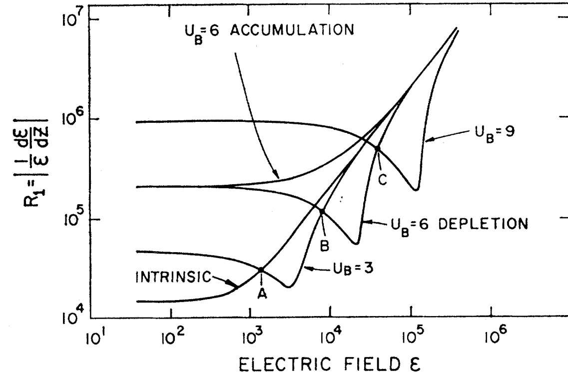

FIG. 1. R_1 versus magnitude of surface electric field $\mathcal{E}$ for four values of impurity concentration for Ge at 300°K. Except for the $u_B=6$ curve, only the depletion region is shown. Curves can be used for n- or p-type material. Points A–C indicate the fields above which it is better to use a sample with the next higher doping level shown.

charge regions. We note that for a given $|\mathcal{E}|$, R_1 is always greater for accumulation than depletion. Thus the line shapes in ER experiments will always be better when obtained from depletion layers. Because of the different values of R_1 for accumulation and depletion, the line shapes will not necessarily be of the same form on either side of flat band unless the fields are less than 10^3 V/cm.

The second and most important feature of Fig. 1 is that only for intrinsic material does increasing the field always result in a larger R_1 and consequently a more nonuniform field over a given depth into the semiconductor. As the doping level is increased, R_1 as defined in Eq. (7) has a minimum at higher and higher fields. From Fig. 1 it can be seen that for a given field there will be an optimum doping level. Figure 2 shows the optimum doping versus field. All other doping levels will give larger R_1's at the given field. Since the optimum experimental conditions require R_1 to be as small as possible, it is clear that by proper choice of doping level, one can go to higher fields with less inhomogeneity with extrinsic material. Consider, for example, the four doping levels shown in Fig. 1. For fields larger than the field corresponding to point A, a sample with $u_B=3$ has a smaller value of R_1 than intrinsic material. Likewise, for fields larger than the field at point B, R_1 for a sample

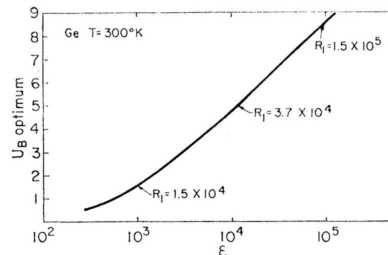

FIG. 2. Optimum doping u_B versus electric field $\mathcal{E}$ for germanium at room temperature. R_1 is given at three points.

[5] K. Zaininger, in *Field Effect Transistors*, edited by J. Wallmark and H. Johnson (Prentice-Hall, Inc., Englewood Cliffs, N. J., 1966), p. 24.

[6] A. Many, Y. Goldstein, and N. B. Grover, *Semiconductor Surfaces* (North-Holland Publishing Co., Amsterdam, 1965), p. 139.

TABLE I. Optimum values of $R_1/|2K|$ for various doping levels and photon energies in germanium at 300°K.

Doping level	Optimum field (V/cm)	$R_1/\|2K\|$ 0.8 eV	2.2 eV	4.0 eV
$N_D=5\times10^{14}/cm^3$ ($u_B=3$)	3.1×10^3	0.063	0.018	0.01
$N_D=1\times10^{16}/cm^3$ ($u_B=6$)	2.2×10^4	0.165	0.048	0.027
$N_D=2\times10^{17}/cm^3$ ($u_B=9$)	1.2×10^5	0.56	0.16	0.09

with $u_B=6$ is always less than R_1 for $u_B=3$ or $u_B=0$. Beyond the field at point C, $u_B=9$ is superior to the three lower doping levels. At the minimum of the $u_B=9$ curve, which occurs at $\mathcal{E}=1.3\times10^5$ V/cm, R_1 is approximately 14 times smaller than R_1 for intrinsic material at the same field. While it should be emphasized that each field has a different optimum u_B, for practical purposes, a given doping can be used over a range of fields.

The factor R_2 depends on the form of the line shape as a function of the photon energy and electric field. Experimental observations[7] at the direct edge and above[8] have shown that a strong excitonic component is present in all line shapes. However, since there are no explicit expressions which can be used for the exciton, we have calculated R_2 for the one-electron line shapes[9] used by Aspnes and Frova in their calculation of $\langle\Delta\epsilon\rangle$. We find that R_2 depends only on η where $\eta=(\hbar\omega-Eg)/\hbar\theta$ and $\theta=[(e\mathcal{E})^2/2\mu\hbar]^{1/3}$. For $-3<\eta<1.5$, that is, close to the critical point, $R_2(\eta)$ is of the order of unity. For $\eta>1.5$, R_2 increases monotonously to about 10 at $\eta=4$. Actually any thermal broadening will reduce R_2, so that these values represent an upper limit for the one-electron theory. Therefore, assuming $R_2\simeq1$, the uniform-perturbation approximation will be valid when $R_1/|2K|\ll1$ in regions near the critical point. For $\eta>1.5$, increasing inhomogeneity should be observed. From Fig. 2 of the work of Aspnes and Frova,[1] we estimate that with $R_2\simeq1$, $R_1/|2K|\simeq0.1$ is a rough upper limit for the validity of the uniform-perturbation approximation.

In Table I we have given $R_1/|2K|$ at 0.8, 2.2, and 4 eV for Ge at three different fields corresponding to the minima of the $u_B=3$, 6, and 9 curves of Figs. 1 and 2. This quantity is the fractional change in the electric field over an "effective" penetration depth. The effective penetration depth $1/|2K|=[(4\pi n/\lambda)^2+\alpha^2]^{-1/2}$ may be much smaller than the actual penetration depth $1/\alpha$ if λ/n is small enough. For example, in Ge at the fundamental edge, $1/\alpha\simeq3\times10^4$ Å while $1/|2K|\simeq400$ Å.

From Table I and Fig. 1, we see that for fields of the order of 3.1×10^3 V/cm a doping level of $u_B=3$ will give the uniform-perturbation approximation at the direct edge in Ge. At higher fields ($>2\times10^4$) both intrinsic and extrinsic samples give $R_1/2|K|>0.1$ at the direct edge. At higher energies where the effective penetration depth is smaller, larger fields are possible with other doping levels.

Table II gives $R_1/|2K|$ at 2.2 eV for the fields used by Aspnes and Frova[1] in calculating $\langle\Delta\epsilon\rangle$ for intrinsic Ge. Also given are the optimum values of $R_1/|2K|$ for the same fields found by interpolation of the minima of Fig. 1. For an experiment conducted at field strengths of $\mathcal{E}=6.5\times10^3$, 3×10^4, and 2.5×10^5 V/cm, Table II indicates that the inhomogeneity in intrinsic Ge is approximately 3, 8, and 21 times worse, respectively, than that for the optimum dopings. It should be obvious from the figures and Table II that there will be large mixing effects when one uses intrinsic Ge over such a wide range of fields.

TABLE II. $R_1/|2K|$ at 2.2 eV in germanium at 300°K.

Field (V/cm)	$R_1/\|2K\|$ Intrinsic	Optimum doping	Improvement ratio
6.5×10^3	0.11	0.033	3.3
3.0×10^4	0.53	0.063	8.4
2.5×10^5	4.4	0.21	21

TABLE III. $R_1/|2K|$ for germanium at 2.2 eV using a sample with an impurity concentration of $N_D=1\times10^{16}/cm^3$ ($u_B=6$).

Field (V/cm)	$R_1/\|2K\|$
0.5×10^4	0.15
1.1×10^4	0.10
2.2×10^4	0.048
3.1×10^4	0.20

III. COMMENTS

We have shown that by proper choice of doping level, one can minimize the inhomogeneity for a given magnitude of the surface field. While $R_1R_2/|2K|$ cannot be made <0.1 for certain fields and photon energies, the improvement in the line shapes in such cases should still be significant.

Since it is difficult for an experimentalist to use a large variety of samples, Table III gives a few points from the $u_B=6$ curve of Fig. 1, and shows the range over which the uniform-perturbation approximation is satisfied near a critical point.

We also note from Eq. (7) that R_1 is proportional to the differential space-charge capacitance[10]

$$C_{sc}=\frac{q}{kT}\frac{dQ_{sc}}{d(u_S-u_B)}=\frac{\kappa\epsilon_0}{L_D}\frac{dF(u_S,u_B)}{du_S}=\kappa\epsilon_0R_1. \quad (8)$$

[7] Y. Hamakawa, P. Handler, and F. Germano, Phys. Rev. **167**, 709 (1968).
[8] K. Shaklee, J. Rowe, and M. Cardona, Phys. Rev. **174**, 828 (1968).
[9] D. E. Aspnes, Phys. Rev. **153**, 972 (1967).
[10] Reference 5, p. 27.

A measurement of the minimum in C_{sc} at zero current locates the minimum in R_1 and thus the optimum field.

For other semiconductors or germanium at other temperatures the dielectric constant κ and the intrinsic carrier concentration n_i will be different. Figures 1 and 2 can still be used with the following scale changes:

$$R_1(\kappa,n_i,T)=R_1(\text{Ge, }300°\text{K})\times(1.38\times10^{-5})\times(n_i/\kappa T)^{1/2},$$

$$\mathcal{E}_s(\kappa,n_i,T)=\mathcal{E}_s(\text{Ge, }300°\text{K})\times(4.63\times10^{-8})\times(n_iT/\kappa)^{1/2},$$

where $\kappa=16$ and $n_i=2.5\times10^{13}/\text{cm}^3$ for Ge at $T=300°$K.

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de Haas–van Alphen Effect in $AuGa_2$

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New de Haas–van Alphen data on the metallic fluorite compounds $AuGa_2$ and $AuIn_2$ are presented. Several new frequency branches have been observed, including two in $AuGa_2$, which are tentatively ascribed to electrons in the fifth zone. The results are in general agreement with recent theoretical calculations by Switendick, which predict that the second zone is full in $AuGa_2$.

IN what has recently been termed "the $AuGa_2$ dilemma"[1] it has been observed that, of the three metallic compounds $AuAl_2$, $AuGa_2$, and $AuIn_2$, which have the fluorite structure, $AuGa_2$ shows anomalous properties in the magnetic susceptibility, Knight shifts, nuclear spin-lattice relaxation rate, and thermoelectric power,[2] whereas the de Haas–van Alphen (dHvA) results[3] to date show a remarkable similarity between the three Fermi surfaces and the nearly free-electron (NFE) model. More recently, superconducting critical points, heat capacities, and magnetic susceptibilities of $AuGa_2$ and its dilute alloys with palladium have been studied,[4] and further measurements on nuclear-magnetic-resonance measurements have been performed.[5] Switendick[5,6] has performed augmented-plane-wave calculations of the band structure of these compounds and has proposed that some of the above anomalous properties may be related to his result that, of the above three compounds, the second band is full only in $AuGa_2$.

In this note we present new dHvA data observed in high-resistance-ratio ($\sim$700) $AuGa_2$ crystals using high (up to 95 kG) magnetic fields. Previous dHvA data are confirmed, and the new data are consistent with the interpretation that in $AuGa_2$ the second band is fully occupied at 4.2°K. Furthermore, there is strong evidence for the existence of a fifth-zone surface which is predicted by Switendick's calculations.[6]

In Fig. 1, we show the third and fourth zones of the (NFE) model,[3] along with the extremal cross sections in the principal crystallographic directions. In Fig. 2, we show the experimental results for H in the (110), for the areas of the smaller extremal orbits, and in Fig. 3, results for all orbits in (100) and (110) compared with the results of Stafleu and van't Hof-Grootenboer[7] for $AuIn_2$ for a sample with a much lower residual resistance ratio. Areas are measured in terms of $(2\pi/a)^2$ throughout, where a is the lattice parameter. We have assigned areas to orbits according to the NFE labels in Fig. 1. In addition to results which confirm those of Jan *et al.*,[3] we present the following new data: (a) the assigned arms B_3, B_4, C_3'', and A_3, which confirm the essential one-to-

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