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## Magnetic field dependence of cyclotron resonance linewidths in Ge and Si by a projection technique

Nam Lyong Kang, Kyu Soon Bae, Chang Ho Choi, Youn Ju Lee, Jung Young Sug, Jung Ho Kim and Sang Don Choi

Department of Physics, Kyungpook National University, Taegu 702-701, Seoul, Korea

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**Abstract.** The magnetic field dependence of cyclotron resonance linewidths is examined theoretically on the basis of the projection technique. It is shown that in the quantum limit of pure Ge and Si the widths increase with the magnetic field, and the result for Ge agrees quite well with the existing experimental data.

### 1. Introduction

It is well known that under the influence of a magnetic field applied along the  $z$  axis, the electronic state in the bulk of a crystal is quantized in the  $x$ - $y$  plane. If, in addition, an electromagnetic wave enters the system, an electron absorbs the proper photon energy to make an optical transition to one of the upper levels, either in the same valley or in the others. Among the many kinds of optical transition, the cyclotron transition has received considerable attention recently, the reason being that the cyclotron transition lineshape is affected by the scattering mechanisms. If we are interested in the intrinsic semiconductors, phonon scatterings are known to be most popular. Investigation of linewidths in these materials gives information about the electronic behaviour. Experimentally, in order to see good resonance lineshapes, low temperatures and high magnetic fields are required. Nowadays, due to the rapid progress in low-temperature technology, getting high fields even far above 10 T, which produce excellent Landau splittings in semiconductors, is possible.

In 1983, by utilizing the projection technique presented by Argyres and Sigel (Argyres and Sigel 1974), the present group introduced a theory of cyclotron resonance lineshapes due to electron-phonon interactions (Choi and Chung 1983). Since then, the theory has been reviewed (Ryu *et al* 1985) by using Kawabata's technique (Kawabata 1967). However, applications to real systems could only be made in the limited scheme (Ryu *et al* 1990) since numerical as well as analytical calculations encounter mathematical difficulties, and thus the validity of the theory could not be checked easily. Nowadays, however, these difficulties have been removed due to improvements in computer technology. The purpose of this paper is to demonstrate the validity of the projection technique by comparing numerical values of the width with existing experiments.

In this paper we restrict ourselves to the case of the three-dimensional electron systems in Ge and Si, for which the deformation potential phonon scattering is dominant, because this case is easily solved. In comparison with low-dimensional systems, however, very little attention has been paid to this three-dimensional case, the reason being that low-dimensional systems are known to be more attractive from the technological point of view (Ando

and Uemura 1974, Wu and Peeters 1992). Nonetheless, a study of the three-dimensional behaviour of electrons in solids is believed to be important in the sense that an understanding of high symmetry may precede that of low symmetry.

The paper is organized as follows. In section 2 we briefly review the theory and change the formula into an easy-to-manage form. Here only the MWC scheme is taken into account, since the formula in this scheme is more similar to that of other authors (Lodder and Fujita 1968, Suzuki and Dunn 1982). It is to be noted that the difference between the so-called MWC (moderately weak coupling) and EWC (extremely weak coupling) schemes originates from an application of the cyclic relation  $\text{Tr}(ABC) = \text{Tr}(CAB)$  in the calculation of the expectation value of the current, where 'Tr' denotes the trace. Since the matrix elements of the operators  $A$ ,  $B$  and  $C$  involve the phonon states as well as the electron states,  $\text{Tr}(ABC)$  and  $\text{Tr}(CAB)$  yield different results in general. Thus we obtained the two formulas (the MWC formula and the EWC formula) for lineshapes (Ryu *et al* 1985). It is expected that this difference does not appear if we include all the higher-order parts which have been neglected here.

In section 3 we apply the theory to calculate the linewidth in Ge and Si in the quantum limit. The magnetic field dependence of the width will be compared with the experimental result of Kobori *et al* (1990) and the theoretical result of Cho *et al* (1994). Note that the theory of Cho and Choi, presented more recently, is based on a different method (Argyres and Sigel 1974).

Section 4 is devoted to discussions and concluding remarks.

## 2. Review of the theory

### 2.1. The theory

For a static magnetic field  $B$  applied in the  $z$  direction, the single electron energy eigenvalue  $E_\alpha$  corresponding to the eigenstate  $|\alpha\rangle = |N, k\rangle$ ,  $N$  being the Landau level index and  $k$  the electron wavevector, is given by

$$E_\alpha \equiv E(N, k_z) = (N + 1/2)\hbar\omega_c + \hbar^2 k_z^2 / 2m \quad (1)$$

where  $\omega_c \equiv eB/m_c$  is the cyclotron frequency,  $m_c$  and  $m$  being the cyclotron and density-of-states effective masses, respectively. If the background is a phonon field, the scattering potential is given by

$$V = \sum_q (\gamma_q b_q + \text{HC}). \quad (2)$$

Here

$$\gamma_q = C_q \exp(iq \cdot r) \quad (3)$$

where  $b_q$  ( $b_q^\dagger$ ) is the annihilation (creation) operator for a phonon of energy  $\hbar\omega_q$  and momentum  $\hbar q$ , and  $C_q$  the interaction parameter. The phonon Hamiltonian is given by

$$H_p = \sum_q \hbar\omega_q (b_q^\dagger b_q + 1/2). \quad (4)$$

Now if a microwave of frequency  $\omega$  is applied, the absorption power, which is proportional to the absorption coefficient, is given by (Kawabata 1967)

$$P(\omega) \propto \text{Re}[\sigma_{+-}(\omega)] \quad (5)$$

where 'Re' denotes 'the real part of' and the optical conductivity tensor  $\sigma_{+-}(\omega)$  is given, in the Kubo formalism, as (Choi and Chung 1983)

$$\sigma_{+-}(\omega) = \left(\frac{1}{\omega_c}\right) \sum_{\alpha} [f(E_{\alpha}) - f(E_{\alpha} + \hbar\omega_c)] |j_{\alpha}^{+}|^2 [i\hbar(\omega - \omega_c) + \hbar\tilde{\Gamma}_{\alpha}(\omega)]^{-1}. \quad (6)$$

Here the collision factor  $\tilde{\Gamma}_{\alpha}(\omega)$  will be explained later and  $f(E_{\alpha}) = \{\exp[\beta(E_{\alpha} + E_c - E_f(T))] + 1\}^{-1}$  is the Fermi distribution for electrons,  $E_c$  being the conduction band minimum and  $E_f(T)$  the Fermi energy given by (Cho and Choi 1994)

$$E_c - E_f(T) = \frac{1}{2}E_g(0) - \kappa T^2 / [(T + \xi)/2] - \frac{3}{4}k_B T \ln(\bar{m}/m) \quad (7)$$

where  $E_g(T)$  is the energy gap at the temperature  $T$ ,  $\kappa$  and  $\xi$  are characteristic constants of the material and  $\bar{m}$  is the density-of-states mass of the hole. The reason why the density-of-states masses are used instead of the isotropic effective mass is that the band structure of Ge and Si is almost ellipsoidal. The current operator  $j^{+}$  is defined as  $j^{+} \equiv j_x + ij_y$ ,  $j$  being the single electron current operator, the matrix element of which is given as  $j_{\alpha}^{+} \equiv \langle \alpha + 1 | j^{+} | \alpha \rangle = -ie [2\omega_c(N + 1)/m]^{1/2}$ . The collision factor  $\tilde{\Gamma}_{\alpha}(\omega)$  in (6), sometimes called the lineshape function, is determined by the scattering mechanism. For phonon scatterings, it is given by (Choi and Chung 1983)

$$i\hbar\tilde{\Gamma}_{\alpha}(\omega) = \sum_q |C_q|^2 [(1 + n_q)\tilde{X}_1(\alpha, q) + n_q\tilde{X}_2(\alpha, q)]. \quad (8)$$

Here  $n_q$  is the Planck distribution function for phonons, given by  $n_q = [\exp(\beta\hbar\omega_q) - 1]^{-1}$  and

$$\begin{pmatrix} \tilde{X}_1(\alpha, q) \\ \tilde{X}_2(\alpha, q) \end{pmatrix} = \left( \sum_{\beta \neq \alpha} (\hbar\omega^- - E_{\alpha+1} + E_{\beta} \pm \hbar\omega_q)^{-1} + \sum_{\beta \neq \alpha+1} (\hbar\omega^- + E_{\alpha} - E_{\beta} \mp \hbar\omega_q)^{-1} \right) K(N, N'; t) \delta_{k', k \pm q_z} \quad (9)$$

where  $\omega^- \equiv \omega - ia$  ( $a \rightarrow 0^+$ ) and the electron states are expressed as  $|\alpha + 1\rangle \equiv |N + 1, k\rangle$  and  $|\beta\rangle = |N', k'\rangle$ . The upper and lower signs on  $\hbar\omega_q$  correspond to  $\tilde{X}_1$  and  $\tilde{X}_2$ , respectively. The  $K$  matrices in (9) are defined as (Argyres and Sigel 1974)

$$K(N, N'; t) = \begin{cases} -\frac{N!}{N'!} t^{N'-N} \exp(-t) L_N^{(N'-N)}(t) L_{N+1}^{(N'-N-1)}(t) & N < N' \\ \frac{N!}{(N+1)!} t^{N-N'+1} \exp(-t) L_N^{(N-N')}(t) L_{N'}^{(N-N'+1)}(t) & N \geq N' \end{cases} \quad (10)$$

where  $t \equiv \hbar q_{\perp}^2 / eB$  with  $q_{\perp} = (q_x^2 + q_y^2)^{1/2}$  and  $L_n^{(m)}(t)$  is the associated Laguerre polynomial.

## 2.2. The lowest-order approximation

Now we confine ourselves to the case of the quantum limit in which  $\hbar\omega_c \gg k_B T$ . We then may assume that only the lowest Landau level is occupied by the electrons. In other words, the transition between the states  $\alpha = (0, k)$  and  $(1, k)$  is dominant. Then we have

$$\tilde{P}(\omega) \propto \frac{1}{\omega_c} \int_{-\infty}^{\infty} dk_z \frac{[f\{E(0, k_z)\} - f\{E(1, k_z)\}]\gamma(\omega, \omega_c; k_z)}{(\omega - \omega_c)^2 + [\gamma(\omega, \omega_c; k_z)]^2}. \quad (11)$$

Considering the spin degeneracy for electrons, and utilizing  $\text{Im}(x - ia)^{-1} = \pi\delta(x)$ , where 'Im' denotes 'the imaginary part of', we have

$$\hbar\gamma(\omega, \omega_c; k_z) = 2V_0 \int \frac{d^3q}{(2\pi)^3} |C_q|^2 [(1 + n_q)\tilde{X}_1 + n_q\tilde{X}_2] \quad (12)$$

where  $V_0$  is the volume of the system and, by taking only the most dominant terms, the terms  $\tilde{X}_1$  and  $\tilde{X}_2$  are given by

$$\begin{aligned} \begin{pmatrix} \tilde{X}_1 \\ \tilde{X}_2 \end{pmatrix} = \pi \left( \sum_{\beta \neq (1, k)} \delta[\hbar\omega + E(0, k_z) - E(N', k_z + q_z) \mp \hbar\omega_q] \right. \\ \left. + \sum_{\beta \neq (0, k)} \delta[\hbar\omega - E(1, k_z) + E(N', k_z + q_z) \pm \hbar\omega_q] \right) K(0, N'; t). \end{aligned} \quad (13)$$

The  $K$  matrices appearing in (13) are now

$$K(0, 0; t) = t \exp(-t) \quad K(0, N'; t) = (-1/N'!) t^{N'} \exp(-t) L_0^{(N')}(t) L_1^{(N'-1)}(t)$$

for  $N' > 0$ . Note that in (13)  $\beta \neq (1, k)$  implies that  $N' \neq 1$  and/or  $q_z \neq 0$  and  $\beta \neq (0, k)$  means  $N' \neq 0$  and/or  $q_z \neq 0$ .

## 3. Linewidths in Ge and Si

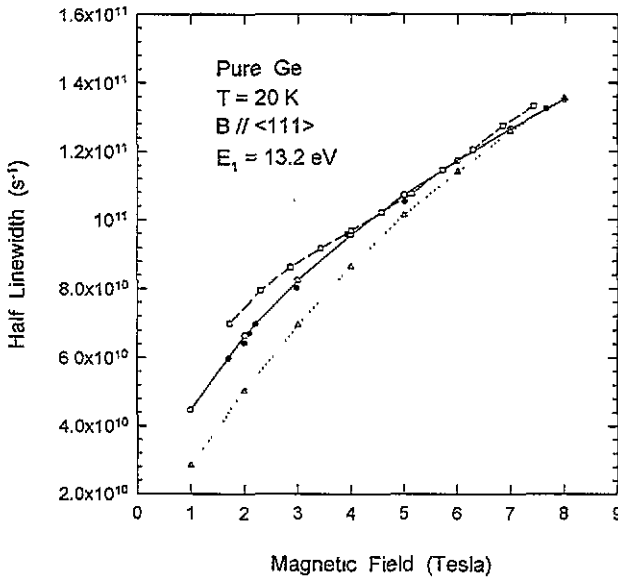
In this section we will calculate the linewidths in Ge and Si in the quantum limit. It is well known that for pure Ge and Si the deformation potential scattering is dominant. According to Bardeen and Shockley (1950),  $C_q$  for the deformation potential scattering is given by

$$|C_q|^2 = \frac{\hbar E_1^2 q}{2\rho s V_0} \quad (14)$$

where  $q \equiv |q|$ ,  $\rho$  is the mass density and  $s$  the speed of sound in the material. The deformation potential constant  $E_1$  is usually adopted as the fitting parameter when any comparison of the theory with the existing experiment is made. It is also known that in these materials the long-wavelength acoustic phonons with  $\omega_q = sq$  play the most important part.

Furthermore, we make an approximation that the  $q$  in the delta functions in (13) is replaced by  $q_{\perp}$ . It is known that this approximation is quite acceptable in the quantum limit since  $q = q_{\perp}(1 + q_z^2/q_{\perp}^2)^{1/2}$  and  $q_z^2/q_{\perp}^2 \simeq k_B T/2\hbar\omega_c \simeq 0$ . If all the physical constants of Ge and Si are known, we can obtain the lineshapes from (11)–(13), which give the linewidths.

As pointed out in the last section, the band structure of Ge and Si can be considered to be ellipsoidal in approximation. For  $B \parallel \langle 111 \rangle$  in Ge we have  $m_c = 0.082 m_0$ ,  $m = 0.22 m_0$  and  $\bar{m} = 0.35 m_0$ , where  $m_0$  is the free electron mass. The other constants are  $\rho = 5.36 \text{ g cm}^{-3}$ ,  $s = 5.94 \times 10^5 \text{ cm s}^{-1}$ ,  $\mathcal{E}_g(0) = 0.744 \text{ eV}$ ,  $\kappa = 4.77 \times 10^{-4} \text{ eV K}^{-1}$  and  $\xi = 235 \text{ K}$ . With these constants inserted into (1), (7), (13) and (14) and carrying out the integration in (11) we obtain the lineshapes, from which the width can be measured. From figure 1 we see that for various frequencies  $\omega = 2.14 \times 10^{12}$ ,  $4.28 \times 10^{12}$ ,  $6.43 \times 10^{12} \text{ s}^{-1}$ , ... ( $\lambda = 879, 440, 293 \text{ } \mu\text{m}$ , ...), at a temperature of 20 K, and with  $E_1$  (the fitting parameter) equal to 13.2 eV, the magnetic field dependence of the width in Ge agrees quite well with the experiment of Kobori *et al* (1990) and with the theoretical data of Cho *et al* (1994).



**Figure 1.** Magnetic field dependence of cyclotron resonance half-linewidths in pure germanium for various wavelengths and a temperature of 20 K. Open circles linked by full curves denote the present theoretical result; full circles show the experimental data of Kobori *et al* (1990). The squares linked by the broken curves denote the theoretically calculated data of Cho *et al* (1994) and the triangles linked by dotted curves denote the theoretical data of Kobori *et al* (1990).

Now for Si, we have  $m_c = 0.19 m_0$ ,  $m = 0.33 m_0$ ,  $\bar{m} = 0.58 m_0$ ,  $\rho = 2.34 \text{ g cm}^{-3}$ ,  $s = 9.03 \times 10^5 \text{ cm s}^{-1}$ ,  $\mathcal{E}_g(0) = 1.17 \text{ eV}$ ,  $\kappa = 4.73 \times 10^{-4} \text{ eV K}^{-1}$  and  $\xi = 636 \text{ K}$ . For various frequencies  $\omega = 9.27 \times 10^{11}$ ,  $1.85 \times 10^{12}$ ,  $2.78 \times 10^{12} \text{ s}^{-1}$ , ... ( $\lambda = 2034, 1017, 679 \text{ } \mu\text{m}$ , ...), at a temperature of 20 K, and with  $E_1 = 9.3 \text{ eV}$ , the result is shown in figure 2. The experimental data are available only for  $\omega = 3.67 \times 10^{12} \text{ s}^{-1}$  ( $\lambda = 513 \text{ } \mu\text{m}$ ). By fitting the theory with the experiment for this value, we have  $E_1 = 9.3 \text{ eV}$ . As shown in figure 2, the magnetic field dependence of the width is in qualitative agreement with the theoretically predicted data of Kobori *et al* (1990).

#### 4. Discussions and concluding remarks

In the last section we saw that the half-linewidths of cyclotron resonance in pure Ge and Si increase with the magnetic field. The tendency of the increase in the width in the quantum

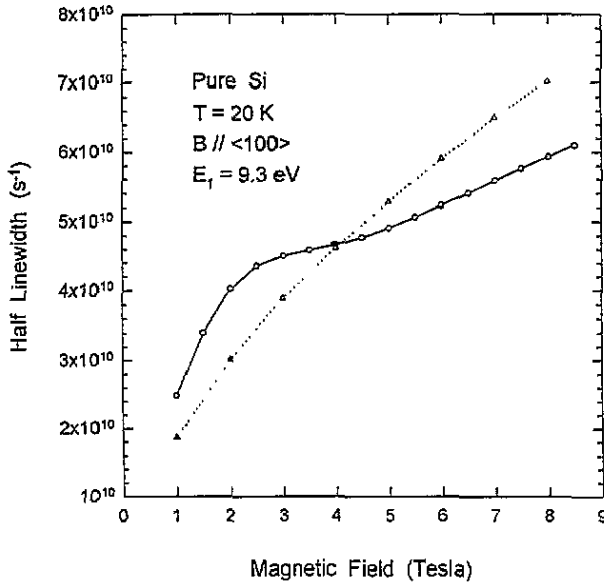


Figure 2. Magnetic field dependence of cyclotron resonance half-linewidths in pure silicon for various wavelengths and a temperature of 20 K. Open circles linked by full curves denote the present theoretical result. Triangles linked by the dotted curves denote the theoretically predicted data of Kobori *et al* (1990). The full circle (almost overlapped by an open circle and a triangle showing the theoretical result at 3.96 T) is the experimental datum of Kobori *et al* (1990).

limit for deformation potential phonon scatterings with the magnetic field was predicted analytically by some early theories (Meyer 1962, Arora and Spector 1979, Suzuki *et al* 1980, Suzuki and Dunn 1982). Later the tendency for Ge was confirmed by the experiment of Kobori *et al* (1990), who also succeeded in obtaining the theoretically calculated data for Ge in comparison with their experiment, convincing us of the tendency. More recently, Cho *et al* (1994) got their data by utilizing the isolation-projection technique introduced by Argyres and Sigel (1974), as shown in figure 1. The theoretical results of Cho *et al* (1994) and of Kobori *et al* (1990) agree quite well with experiment in the high-magnetic-field region. We see that the present result is more satisfactory, compared with the previous ones.

Unfortunately, the result for Si could not be checked due to the lack of experimental data. As shown in figure 2, only one datum is available for Si. However, we see that our theoretical result agrees qualitatively well with the theoretically predicted result of Kobori *et al* (1990), showing that the width in Si also increases with the magnetic field.

We have adopted the deformation potential constant  $E_1$  as the fitting parameter, as in the works of other authors (Cho *et al* 1994, Stradling and Zhukov 1966, Ito *et al* 1964, Murase *et al* 1970). The values obtained in this work are  $E_1 = 13.2$  eV for Ge and  $E_1 = 9.3$  eV for Si, which are similar to those of the other authors.

In conclusion, we see that the projection technique successfully explains the tendency of increase in the cyclotron resonance linewidths in Ge and Si with the magnetic field in the quantum limit. In other words, we may claim that the projection technique yields successful results in magneto-optical transitions in solids.

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