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Calculation of the anisotropic mobility in (110) AlAs quantum wells at zero temperature

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We calculate the mobility of the two-dimensional electron gas as realized in (110) AlAs quantum wells at zero temperature. In this structure the mass is strongly anisotropic which gives rise to an anisotropic mobility. By using a theoretical approach developed by Tokura [Phys. Rev. B **58**, 7151 (1998)] we numerically calculate the anisotropic mobility. We study impurity scattering in quantum wells having an ellipsoidal Fermi surface. We find that increasing the electron density and/or the well width results in reduction of the anisotropy of the mobility while the anisotropy in the scattering time is increased. A strong dependence of the mobility anisotropy on the impurity position is predicted. Excellent agreement with a recently published experimental result is found under the assumption that impurities are located at the edge of the quantum well.

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An anisotropic Fermi surface and/or an anisotropic disorder lead to anisotropic transport properties in semiconductors. This is well known for three-dimensional semiconductors [1]. There exists some theoretical [2] and experimental [3] work concerning anisotropic transport properties of the two-dimensional electron gas in silicon (110), where the effective mass is anisotropic, but no comparison between experiment and theory was performed. More recently Tokura [4] has published a theoretical work on anisotropic scattering potentials and anisotropic transport properties in the two-dimensional electron gas. It is known that a scattering problem for an anisotropic effective mass and an isotropic scattering potential can be reduced to that of an isotropic effective mass and an anisotropic scattering potential [1].

Transport properties of the two-dimensional electron gas in (100) AlAs quantum wells (QW's) have been studied extensively in experiment [5] and theory [6]. In (100) AlAs QW's the effective mass and the mobility are isotropic. Recently, electronic properties of an anisotropic two-dimensional electron gas as realized in (110) AlAs QW's have been reported [7]. In this system, for large enough well width $w > 53$ Å only one conduction-band valley is occupied with an elliptic Fermi surface and longitudinal and transverse effective masses of $m_l = 1.1m_e$ and $m_t = 0.2m_e$, respectively, where m_e is the free electron mass. The ratio of the mobilities along the main symmetry axes was found to be 2.8, much smaller than the corresponding effective mass ratio of 5.5 [8]. This experimental result motivated us to study anisotropic transport in two-dimensional electron gases. In the present paper we apply the theory [4] to single-valley anisotropic (110) AlAs QW's and present numerical results for the anisotropic mobility at zero temperature in the case of impurity scattering.

In the following we choose the x and y coordinate axes along the two symmetry axes in the (110) AlAs plane and the z-axis along the [110] confinement direction. In these coordinates the in-plane effective mass tensor of the two-dimensional electron gas becomes diagonal with two effective masses $m_x = m_l$ and $m_y = m_t$ ($m_x > m_y$). We consider a QW with infinite barriers at $z = 0$ and $z = w$ and the electron gas is located in this QW at $0 < z < w$. We suppose that there is disorder due to randomly distributed charged impurities of density N_I in the xy-plane at a distance z_I from this plane. For $z_I = w/2$ the impurities are located at the center of the QW and for $z_I = 0$ or $z_I = w$ the impurities are located at the edge of the QW. These two cases will be discussed in the following. Coulomb interaction effects are treated within the random-phase approximation which leads to conventional screening of the random potential by a q-dependent dielectric function [9]. The unscreened averaged random potential is described by $<|U(q)|^2> = N_I[2\pi e^2 F_I(q, w, z_I)/q\varepsilon_L]^2$. $F_I(q, w, z_I)$ is the form factor depending on the position of impurities and the width of the well. It was calculated before for a Silicon QW [10]. ε_L is the dielectric constant of the background dielectric material and for AlAs we use $\varepsilon_L = 10.16$ [8]. The Fourier transform of the interaction potential is given by $V(q) = 2\pi e^2 F_C(q)/\varepsilon_L q$ with the

form factor $F_C(q)$ due to the finite width. This form factor also can be found in Ref.[10].

The theoretical approach developed in Ref.[4] represents a transport theory for anisotropic scattering potentials of electrons in two dimensions with an isotropic mass. In the present paper we consider charged impurities, for which the scattering potential is isotropic, and electrons with an anisotropic kinetic energy, due to the anisotropic mass. When the anisotropic kinetic energy of the electron gas is transformed, via a Herring-Vogt like transformation, to an isotropic form, the initially isotropic screened Coulomb scattering potential becomes anisotropic. Then we can apply the theory of Ref.[4] to calculate the two scattering times τ_x and τ_y in order to describe the anisotropic transport properties.

With the help of the Herring-Vogt like transformation one can write the kinetic energy of a particle $E(k_x, k_y) = \hbar^2 k_x^2/2m_x + \hbar^2 k_y^2/2m_y$ as $E(k) = E_F[(k_x/k_x^F)^2 + (k_y/k_y^F)^2] = E_F \widetilde{\mathbf{k}}^2$ with the dimensionless vector $\widetilde{\mathbf{k}}$ and the Fermi energy $E_F = (\hbar k_x^F)^2/2m_x = (\hbar k_y^F)^2/2m_y$ [12], see Fig.1. The screened scattering

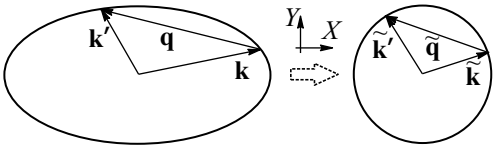

Fig.1. Illustration of the Herring-Vogt like transformation of the elliptic Fermi surface to the spherical Fermi surface

potential due to the impurities is isotropic and depends only on $|\mathbf{q}| = |\mathbf{k} - \mathbf{k}'| = q$. This variable is transformed to $|\widetilde{\mathbf{q}}| = |\widetilde{\mathbf{k}} - \widetilde{\mathbf{k}}'| = \widetilde{q}$. The wave number q is given in terms of $\widetilde{q}$ by $q = \widetilde{q} q_F \sqrt{1 + \alpha \cos(2\psi)}$. Here $\alpha = \frac{m_x - m_y}{m_x + m_y}$ and $q_F = \sqrt{\pi N_S (m_x + m_y)/m_D}$ with the density of state mass defined as $m_D = \sqrt{m_x m_y}$. N_S is the electron density and ψ is the angle between $\widetilde{\mathbf{q}}$ and the x-axis, see Fig.1. Note that in transformed coordinates the scattering potential becomes anisotropic due to the ψ dependence.

Now we shortly describe the theoretical work [4] which we use for our calculations. A relaxation time vector is used to express the non-equilibrium part of the distribution function which enters the Boltzmann equation [11]. It was shown that the corresponding conductivity tensor is diagonal by assuming two symmetry axes of the scattering potential. The input function in this approach is the screened disorder as the scattering function $Q(\widetilde{q}, \psi)$. The unscreened scattering function is calculated in Born approximation and corresponds to the disorder potential which we introduced earlier, however, now expressed with the new variables. $Q(\widetilde{q}, \psi)$ is developed in a Fourier series given by $Q(\widetilde{q}, \psi) = \sum_{m=0}^{\infty} Q_m(\widetilde{q}) \cos(2m\psi)$. The $Q_m(\widetilde{q})$ are given by the inversion, which corresponds to a ψ integral over $Q(\widetilde{q}, \psi)$ weighted by $\cos(2m\psi)$. The two integral-equations for the two scattering times are solved by Fourier expansion. The two solutions are written in terms of two infinite symmetric matrices $K_{l,n}^x$ and $K_{l,n}^y$. These matrices define the scattering times τ_x and τ_y via a matrix inversion. The corresponding mobilities and conductivities, respectively, are given by $\mu_i = e\tau_i/m_i$ and $\sigma_{ii} = N_S e \mu_i$ with $i = x, y$.

For a numerical calculation the infinite symmetric matrixes $K_{l,n}^x$ and $K_{l,n}^y$ must be truncated. We use 5x5 matrixes ($l, n = 1, 2, ..5$) to calculate the scattering times with 4 Fourier elements Q_m ($m = 0, 1, 2, 3$) for the disorder. Note that Q_0 describes isotropic scattering and Q_1 is the most important among the anisotropic terms with $m > 0$. In the isotropic case one finds that $Q_0 \neq 0$ and $Q_m = 0$ for $m > 0$, so that the two scattering times are identical and given by the known expression for an isotropic system [9]. We have checked that even with only two elements Q_m ($m = 0, 1$) one gets already quite accurate results. In the worst case, fulfilled for a large electron density ($N_s = 1 \cdot 10^{12}\,\mathrm{cm}^{-2}$) and large well width ($w = 200$ Å), the truncation of Q_m to two elements gives a 20% underestimated mobility ratio. However, for lower density and smaller well width this approximation becomes more accurate [13].

In Fig.2 the ratio μ_y/μ_x is shown versus electron density for a QW of width $w = 100$Å with impurities at the center of the well. The full line takes all form factors into account. At very low electron density the anisotropic mobility reaches the mass anisotropic value given by $m_x/m_y = 5.5$. This means that in the limit of vanishing electron density the relaxation time is isotropic. This limit was studied before [12]. Finite electron density reduces the anisotropy in the mobility due to screening effects and form factor effects. The importance of the form factors is evident from the dashed and the dotted lines in Fig.2. For the dashed-dotted line we used $F_C = 1$, which results in an underestimation of the anisotropy in the mobility. For the dashed line $F_I = 1$ was used, and the corresponding anisotropy of the mobility is overestimated. The behavior of the mobility anisotropy at low densities can be qualitatively understood [4]. At low wave numbers and for $F_I = 1$ ($F_C = 1$) the scattering probability is an increasing (decreasing) function of q. Therefore, since $k_x^F > k_y^F$, one gets $1/\tau_x > 1/\tau_y$ ($1/\tau_x < 1/\tau_y$) and, correspondingly, $\mu_y/\mu_x > 5.5$ ($\mu_y/\mu_x < 5.5$). We conclude from Fig.2 that the effects coming from both form factors are quan-

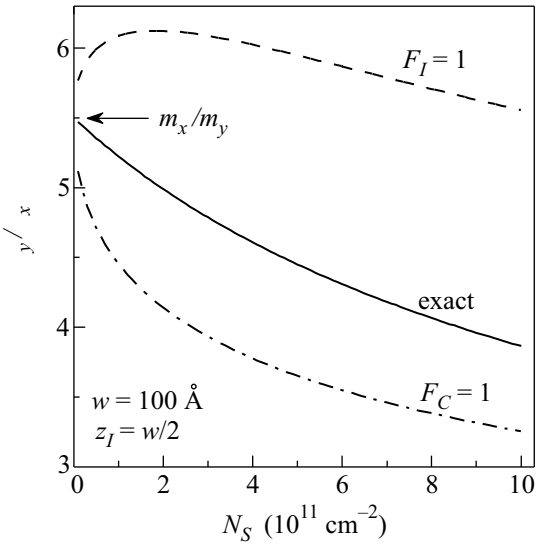

Fig.2. Mobility ratio versus electron density for a (110) AlAs quantum well of width $w = 100$Å with impurities located at the center of the quantum well as the solid line. For the dashed line the impurity form factor is $F_I = 1$. For the dash-dotted line the form factor for the Coulomb interaction is $F_C = 1$. The arrow indicates the mass ratio

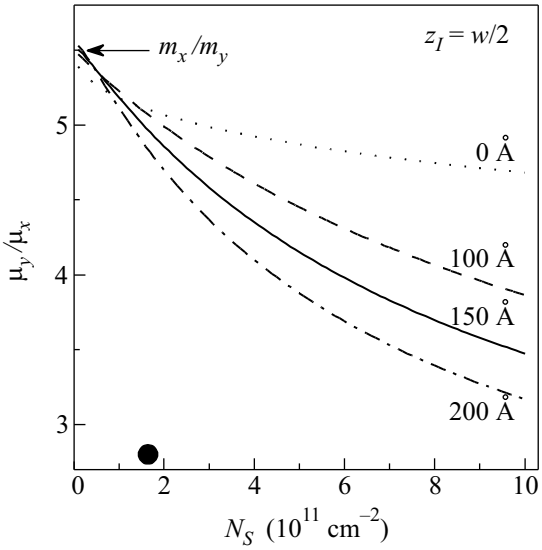

Fig.3. Mobility ratio versus electron density for an AlAs quantum well with impurities located at the center of the quantum well. Results for different well width are shown. The arrow indicates the mass ratio. The solid dot represents the experimental result for the $w = 150$ Å well [7]

titatively very important and any model which neglects these effects cannot account for real QW's.

We note that for short-range disorder, where the unscreened random potential does not depend on q, and for a non-interacting electron gas one finds $\mu_y/\mu_x = m_x/m_y = 5.5$, independent of electron density. In this case the relaxation time is isotropic for all electron densities. For impurity scattering the screened potential is, for small wave number, independent of q and constant. That is why one finds isotropic scattering when k_x^F and k_y^F are approaching zero, which is the case in the low density limit [12]. However, for charged impurity scattering the anisotropy in the mobility decreases with increasing density. This implies that the anisotropy in the scattering times increases with increasing density. The origin of the deviations from $\mu_y/\mu_x = 5.5$ is the q-dependence of the screened random potential which is due to the screening and the two form factors, see Fig.2.

In Fig.3 the ratio μ_y/μ_x is shown versus electron density for different QW widths with impurities in the center of the well. The reduction of the anisotropy in the mobility increases with increasing well width and with increasing density. We repeat that this means that the anisotropy in the scattering times increases strongly with w and with N_S. An ideal electron gas in two dimensions has zero width and the form factors are all equal to one. The calculation for the mobility anisotropy for an ideal electron gas is also shown in Fig.2. Note that the reduction of the anisotropy in the mobility is much smaller than in real quantum wells of finite width. We mention that in experiment [7] with a (110) AlAs QW of width $w = 150$ Å and electron density $N_S = 1.65 \cdot 10^{11}$ cm^{-2}, a mobility ratio $\mu_y/\mu_x = 2.8$ was found. This ratio cannot be explained by impurities at the center of the well: the measured anisotropy of the mobility is too small compared to theory, see the solid dot in Fig.3.

In Fig.4 we show the ratio μ_y/μ_x versus electron density for different QW widths with impurities located at the edge of the well. The mobility anisotropy with impurities at the edge of the QW is smaller than for impurities in the center. With increasing well width the mobility anisotropy increases, as found before in Fig.2. But now the numbers found for μ_y/μ_x are smaller. Our calculated result for $w = 150$ Å shows excellent agreement with the experimental value published recently [7]. From this we conclude that unintentional impurities are located at the edge of the QW, either at one edge or at the two edges. From the absolute value of the mobility reported in experiment $\mu_y = 1.0 \cdot 10^5$ cm^2/V s [7] we obtain the number of impurities $N_I = 1.5 \cdot 10^{10}$ cm^{-2} located at one edge. This is not an unrealistic number for unintentional charged impurities which are accumulated at an edge of the QW. We mention that for the electron gas in (100) AlAs QW it was argued before, comparing theoretical and experimental results, that charged impurities are located at the interface [6].

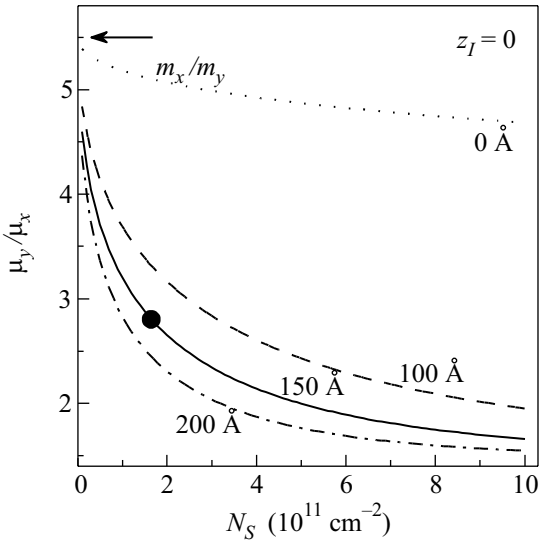

Fig.4. Mobility ratio versus electron density for an AlAs quantum well with impurities located at the edge of the quantum well. Results for different well width are shown. The arrow indicates the mass ratio. The solid dot represents the experimental result for the $w = 150$ Å well [7]

Now we will briefly discuss some assumptions and approximations, which we used in the present paper. For instance, we only showed results for impurity scattering. However, we also have studied interface-roughness scattering for QW's and found that this scattering mechanism increases the mobility anisotropy. For the experimental results on (110) AlAs QW's [7] interface-roughness scattering can be neglected because of the large well width. More results will be published elsewhere [13]. Many-body effects, which can be described by a local-field correction [14], have been neglected in the calculation because no results for anisotropic systems are available in the literature. In the present paper we have studied only an isotropic scattering potential. However, it is known that anisotropic scattering potentials can exist [4]. Such potentials also might contribute to anisotropic transport. Our calculations have been made in lowest order of the disorder and multiple-scattering effects might be important when the impurity concentration increases [6]. Because of the high mobility we expect that multiple-scattering effects are not important for the AlAs QW of Ref.[7]. Concerning the sample structure we stress that the impurity distribution in the sample used in Ref.[7] is not known. This means that our conclusion, that impurities are located at the interface, need to be confirmed.

From our numerical results we conclude that the mobility ratio is very sensitive to the position of impurities. This means that measurements of the mobility anisotropy could be used to get microscopic insight into the impurity distribution of samples. This should be very interesting to samples growers.

We propose to test our theoretical results with additional experiments and we hope that our work initiates such a systematic experimental research. Let us mention that the application of uniaxial stress can be used to make the system anisotropic. We believe that the appearance of an anisotropic mobility in such a system can be used to get information about the disorder in the system.

In conclusion, we calculated the anisotropic mobility in (110) AlAs quantum wells at zero temperature. Our predictions can be tested in experiment and should also apply qualitatively to (110) AlP quantum wells and to (110) $Si_{1-x}Ge_x$ quantum wells.

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