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Intersubband-coupling and screening effects on the electron transport in a quasi-two-dimensional δ -doped semiconductor system

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The effects due to intersubband coupling and screening on the ionized impurity scattering are studied for a quasi-two-dimensional electron system in δ -doped semiconductors. We found that intersubband coupling plays an essential role in describing the screening properties and the effect of ionized impurity scattering on the mobility in a multisubband system. At the onset of the occupation of a higher subband, the screening due to the intersubband coupling leads to a reduction of the small angle scattering rate in the lower subband. We showed that such an effect is significant in a δ -doped quantum well and results in a pronounced increase of the quantum mobility at the onset of the occupation of a higher subband. © 1996 American Institute of Physics.
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I. INTRODUCTION

In the last 2 decades a large amount of work has been published on the impurity scattering mechanism and electron transport properties in quasi-two-dimensional (Q2D) semiconductor systems.¹⁻¹⁰ Screening of the two-dimensional electron gas (2DEG) is the most important factor which affects the ionized impurity scattering. In the seminal article by Stern and Howard⁴ on electron transport in the lowest subband of a 2D system (the quantum limit), it was shown that, by increasing the 2D electron density without changing the number of ionized impurities, the electron mobility could be significantly increased. However, the introduction of small concentrations of impurities into the region of the electron gas degrades the mobility. Masselink⁷ investigated the effect of the dimensionality on the ionized-impurity scattering in semiconductors. He studied the electron mobility in GaAs/AlGaAs quantum-well structures which were doped in different regions of the well and found that the ionized-impurity scattering rate of the Q2D electron gas embedded with identical density of ionized impurities is larger than that of the 3D electron gas with the same density.

When the electron density in a Q2D system is large, typically around 10^{12} cm^{-2} , higher subbands become populated. Several earlier works¹¹⁻¹³ studied multisubband electron transport in Q2D systems taking only two occupied subbands into account. It was shown that, in this case, due to the intersubband scattering, a sharp drop of the electron transport mobility occurs when the second subband becomes occupied. Such an abrupt change in the electron mobility was not found in experiments which was explained by Mori and Ando¹¹ as due to the level broadening effect. Nevertheless, a pronounced decrease in the mobility at the onset of the oc-

cupation of the second subband in a GaAs/AlGaAs heterojunction was observed by Störmer, Gossard, and Wiegmann.¹⁴

The occupation of higher subbands in multisubband electron transport leads to several effects. First, electrons in different subbands may have very different mobilities. Second, more scattering channels are introduced. Beyond the intrasubband scattering, the intersubband scattering becomes crucial in a multisubband system. Third, all the occupied subbands contribute to the screening of the scattering potential and screening due to virtual intersubband transitions may also be appreciable. However, the effects of the intersubband interaction on the ionized impurity scattering have never been worked out completely. Due to the complicated numerics drastic simplifications had been made and therefore the effect of screening on the scattering potential in a multisubband system is still an open question. In the present article we want to address both problems.

In recent years there has been increasing interest in the study of the electron transport properties of the Q2D electron system in δ -doped semiconductors.¹⁵⁻²⁶ Different from modulation-doped heterojunctions, the δ -doped systems are characterized by a rather large electron concentration. Typically, several subbands are occupied and effects resulting from the occupation of several subbands can be studied. Because no interface is present in δ -doped structures and conduction electrons and impurities share the same regions of the system, the ionized impurity scattering is by far the most important scattering mechanism at low temperatures.

This article reports a detailed theoretical study of the screening properties of a 2DEG on the ionized impurity scattering in a multisubband system at zero temperature. The screening effects on the electron subband transport mobility as well as the quantum mobility¹⁰ in δ layers are investigated based on the self-consistent calculation of the electronic

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structure of the system.²⁴ We show that the inclusion of the intersubband coupling of the 2DEG is essential to understand the screening effects in multisubband transport which is limited by ionized impurity scattering.

II. THEORETICAL ANALYSIS

The state of an electron in a Q2D system is described by its eigenenergy $E_n(\mathbf{k}) = E_n + \hbar^2 k^2 / 2m^*$ and the wave function

$$\Psi_{n,\mathbf{k}}(x,y,z) = \psi_n(z) \exp(i\mathbf{k} \cdot \mathbf{r}) / \sqrt{A},$$

where $n=1,2,\dots$, is the subband index, $\mathbf{r}(\mathbf{k})$ the electron position (wave vector) in the xy plane, E_n the subband energy, $\psi_n(z)$ the electron wave function in the z -direction, m^* the electron effective mass, and A the sample area. If we limit ourselves to ionized donor scattering, the transition matrix element between states $|n,\mathbf{k}\rangle$ and $|n',\mathbf{k}'\rangle$ due to the screened scattering potential from the ionized impurity is given by, within the Born approximation,^{24,27}

$$|u_{nn'}(\mathbf{q})|^2 = \left(\frac{2\pi e^2}{\epsilon_0 q} \right)^2 \int dz_i n_D(z_i) \times \left| \sum_{mm'} \epsilon_{nn',mm'}^{-1}(\mathbf{q}) G_{mm'}^{(0)}(q, z_i) \right|^2, \quad (1)$$

with

$$G_{mm'}^{(0)}(q, z_i) = \int_{-\infty}^{\infty} dz \psi_m(z) \psi_{m'}(z) e^{-q|z-z_i|}, \quad (2)$$

where $n_D(z_i)$ is the profile of the ionized impurity, $\epsilon_{nn',mm'}^{-1}(q)$ is the matrix element of the inverse of the dielectric response matrix which describes the screening of the system, $q = (k^2 + k'^2 - 2kk' \cos \theta)^{1/2}$ is the electron momentum transfer due to scattering,

$$k' = [k^2 + (E_n - E_{n'}) 2m^* / \hbar^2]^{1/2},$$

and θ is the scattering angle between $\mathbf{k}$ and $\mathbf{k}'$. The scattering rate for an incident electron in the state $|n,\mathbf{k}\rangle$ scattered into the n' subband per unit angle interval at angle θ is given by^{4,13,27,28}

$$\Gamma_{nn'}(k, \theta) = \frac{m^*}{2\pi\hbar^3} |u_{nn'}(q)|^2. \quad (3)$$

Notice that $\Gamma_{nn'}(k, -\theta) = \Gamma_{nn'}(k, \theta)$.

At zero temperature, only electrons on the Fermi surface contribute to electrical conduction. The quantum mobility $\mu_n^q = e\tau_n^q / m^*$ is determined by the quantum lifetime, or the single particle relaxation time τ_n^q , which is the average scattering time. For a system of N populated subbands the subband quantum lifetime is given by

$$\frac{1}{\tau_n^q} = \sum_{n'=1}^N \int_{-\pi}^{\pi} d\theta \Gamma_{nn'}(k_{Fn}, \theta), \quad (4)$$

where $k_{Fn} = \sqrt{2m^* E_{Fn}} / \hbar$ and $E_{Fn} = E_F - E_n$. On the other hand, the electron subband transport mobility $\mu_n^t = e\tau_n^t / m^*$ is

determined by the transport lifetime or the momentum relaxation time τ_n^t which is obtained by solving the Boltzmann equation.^{11,13,24}

The influence of the intersubband interaction on the electron transport is two-fold:

- (1) Intersubband coupling of the 2DEG affects the screening of the ionized impurity scattering potential, and
- (2) intersubband scattering allows more scattering channels.

The former mechanism is described in Eq. (1) where the transition matrix elements of the screened scattering potential involve all the subbands in the system, even empty subbands. The latter mechanism appears in the transition matrix element $u_{nn'}(q)$ with $n \neq n'$ and only the occupied subbands are involved.

The aim of this work is to study the screening properties in multisubband electron transport. For our purposes, we consider a δ -doped system with zero thickness of the doping layer located at the $z=0$ plane, i.e., $n_D(z_i) = N_D \delta(z_i)$. In this case, the system under consideration is symmetrical about the $z=0$ plane and the intersubband scattering between the two subbands of different parities vanishes. The effect of the intersubband coupling in the screening is more pronounced. Equation (3) reduces to

$$\Gamma_{nn'}(k, \theta) = \frac{1}{t_0} \frac{N_D}{q} |G_{nn'}(q)|^2, \quad (5)$$

with

$$G_{nn'}(q) = \sum_{mm'} \epsilon_{nn',mm'}^{-1}(\mathbf{q}) G_{mm'}^{(0)}(q), \quad (6)$$

where N_D is the ionized donor concentration, $t_0 = \hbar^3 \epsilon_0^2 / 2\pi m^* e^4$ ($t_0 = 0.955 \times 10^{-14}$ s for GaAs), and $G_{mm'}^{(0)}(q) = G_{mm'}^{(0)}(q, 0)$.

The screening of the impurity scattering potential due to the presence of the electron gas can be included within different approximations. The well-known approach is the static random-phase approximation (RPA). The dielectric matrix within the RPA is given by²⁹

$$\epsilon_{nn',mm'}^{\text{RPA}}(q) = \delta_{nn'} \delta_{n'm'} + \frac{2}{a_B q} F_{nn',mm'}(q) \Pi_{mm'}^{(0)}(q), \quad (7)$$

where $a_B = \hbar^2 \epsilon_0 / m^* e^2$ is the effective Bohr radius ($a_B = 99.64$ Å for GaAs), $F_{nn',mm'}(q)$ is the Coulomb form factor,^{11,24} and $\Pi_{mm'}^{(0)}(\mathbf{q})$ is the density response function of the noninteracting system.²⁹ The RPA is the most complicated approach which is used in practical numerical calculations of multisubband electron transport. Due to complications in the numerics often further simplifications are introduced, such as the Thomas–Fermi approximation (TFA)^{13,22} or by only considering the diagonal terms of the RPA dielectric matrix (DRPA).^{30,31} For a multisubband Q2D system, the dielectric function within the TFA is obtained by the long-wavelength limit of the RPA expression,¹³

FIG. 1. The scattering rate as a function of the scattering angle for conduction electrons in the $n=1$ (thick curves) and $n=2$ (thin curves) subbands in Si δ -doped GaAs with total electron density $N_e = 10^{12} \text{ cm}^{-2}$. The solid, dotted, and dashed curves indicate the results obtained within the RPA, TFA, and DRPA, respectively.

$$\epsilon_{nn',mm'}^{\text{TFA}}(\mathbf{q}) = \delta_{nn'}\delta_{n'm'} + \frac{2}{a_B q} \delta_{nn'}\delta_{mm'}\Theta(E_{Fm}), \quad (8)$$

where $\Theta(E)$ is the Heaviside step function. If considering only the diagonal terms of the RPA dielectric matrix, one has

$$\epsilon_{nn',mm'}^{\text{DRPA}}(\mathbf{q}) = \delta_{nn'}\delta_{n'm'}\epsilon_{nn',mm'}^{\text{RPA}}.$$

As a consequence, within the DRPA, we obtain

$$G_{nn'}(q) = G_{nn'}^{(0)}(q)/\epsilon_{nn',nn'}^{\text{RPA}}(q).$$

Notice that, in the quantum limit, the DRPA is equivalent to the RPA within the one subband model.

For the sake of clarity, we consider first the situation of a δ -doped semiconductor where two subbands are populated. In this case, we have $\Gamma_{12} = \Gamma_{21} = 0$ due to the symmetry of the system, i.e., no intersubband scattering takes place. The intersubband interaction influences the electron transport only through the screening. The quantum lifetime and the transport lifetime of the conduction electrons in the two subbands are reduced to

$$\frac{1}{\tau_n^q} = \int_{-\pi}^{\pi} \Gamma_{nn}(k_{Fn}, \theta) d\theta$$

and

$$\frac{1}{\tau_n^t} = \int_{-\pi}^{\pi} \Gamma_{nn}(k_{Fn}, \theta)(1 - \cos \theta) d\theta, \quad (9)$$

with $\Gamma_{nn} = N_D/(t_0 q)|G_{nn}(q)|^2$, for $n=1$ and 2. It is seen that the transport lifetime is different from the quantum lifetime only by the weight $1 - \cos \theta$ in the scattering rate. It implies that the transport mobility is mainly determined by backscattering ($\theta > \pi/2$); but, if intersubband scattering is involved, the above expression for the transport lifetime is not valid. It has a more complicated form which can be obtained from the Boltzmann equation; however, the transport lifetime is still mainly determined by the large angle scattering.

FIG. 2. The quantity G_{nn} as a function of the scattering angle for conduction electrons in the $n=1$ and $n=2$ subbands in Si δ -doped GaAs with $N_e = 10^{12} \text{ cm}^{-2}$. G_{11} (thick solid curve) and G_{22} (thin solid curve) are obtained within (a) RPA and (b) TFA. We also show $\alpha_{11}G_{11}^{(0)}$ (thick dashed curve), $\alpha_{12}G_{22}^{(0)}$ (thick dotted curve), $\alpha_{22}G_{22}^{(0)}$ (thin dotted curve), and $\alpha_{21}G_{11}^{(0)}$ (thin dashed curve).

III. NUMERICAL RESULTS AND DISCUSSION

Figure 1 shows the intrasubband scattering rate $\Gamma_{nn}(k_{Fn}, \theta)$ as a function of the scattering angle for conduction electrons at the Fermi surface in the $n=1$ and 2 subbands in a Si δ -doped GaAs structure with electron density $N_e = 10^{12} \text{ cm}^{-2}$ and background acceptor concentration $n_A = 10^{14} \text{ cm}^{-3}$. In this system the subband Fermi energy of the two populated subbands are $E_{F1} = 25.53 \text{ meV}$ and $E_{F2} = 4.11 \text{ meV}$, respectively. The solid, dotted, and dashed curves show the results obtained within the RPA, TFA, and DRPA, respectively. It is apparent that Γ_{11} , obtained within the different approximations, has a similar overall behavior as a function of θ , it decreases quickly with increasing scattering angle θ or momentum transfer q . At small angle, Γ_{11} within the TFA and DRPA is larger than that within the RPA. The Γ_{22} within the RPA and TFA is considerably smaller than Γ_{11} for small scattering angle, and they do not strongly depend on θ . However, the DRPA leads to $\Gamma_{22}(k_{F2}, \theta) > \Gamma_{11}(k_{F1}, \theta)$ (see the thin and thick dashed curves in Fig. 1) in which the intersubband coupling effect is discarded. Notice that, even though the dielectric function within the TFA is the long-wavelength limit of the RPA, they yield different scattering rates as q approaches zero.

In order to understand the underlying physics of the intersubband coupling effect on the ionized impurity scattering rate, let us consider Eq. (6) within the two subband model which is given by

$$G_{11}(q) = \alpha_{11}G_{11}^{(0)} - \alpha_{12}G_{22}^{(0)}$$

and

$$G_{22}(q) = \alpha_{22}G_{22}^{(0)} - \alpha_{21}G_{11}^{(0)}, \quad (10)$$

TABLE I. The subband quantum mobility in Si δ -doped GaAs.

		μ_1^q	μ_2^q	μ_3^q (cm ² /V s)
Sample W807 $N_e = 1.05 \times 10^{12}/\text{cm}^2$	TFA	909.97	10272.7	
	DRPA	835.11	605.02	
	RPA	1135.5	4471.21	
	Expt	811	3908	
Sample W831 $N_e = 3.08 \times 10^{12}/\text{cm}^2$	TFA	343.44	6461.8	418.39
	DRPA	416.98	382.63	250.17
	RPA	638.57	2984.6	4785.7
	Expt	563	2761	...
Sample W293 $N_e = 4.50 \times 10^{12}/\text{cm}^2$	TFA	300.27	4270.6	480.23
	DRPA	328.21	304.90	230.55
	RPA	524.93	2256.9	4034.6
	Expt	463	2020	4080

where $\alpha_{11} = \epsilon_{11,11}/D$, $\alpha_{12} = \epsilon_{11,22}/D$, $\alpha_{21} = \epsilon_{22,11}/D$, $\alpha_{22} = \epsilon_{22,22}/D$, and $D = \epsilon_{11,11}\epsilon_{22,22} - \epsilon_{11,22}\epsilon_{22,11}$. From the above equations, it is clear that G_{11} (G_{22}) depends both on the $n=1$ ($n=2$) subband and the $n=2$ ($n=1$) subband. They are coupled through the dielectric function. We depict in Fig. 2 the quantity G_{nn} within the RPA and TFA, which correspond to the scattering rate shown in Fig. 1. G_{11} is indicated by the thick solid curves and G_{22} by the thin solid curves. We also show the contributions $\alpha_{11}G_{11}^{(0)}$ and $\alpha_{12}G_{22}^{(0)}$ for G_{11} and $\alpha_{21}G_{11}^{(0)}$ and $\alpha_{22}G_{22}^{(0)}$ for G_{22} . It is clear that the intersubband coupling results in a reduction of the impurity scattering, i.e., $G_{22}^{(0)}$ ($G_{11}^{(0)}$) has a negative contribution to the effective scattering potential for the electron in the $n=1$ ($n=2$) subband. We observe that $G_{11}^{(0)}$ and $G_{22}^{(0)}$ contribute on equal footing to the small angle scattering of the electron transport in the $n=1$ subband; but, for $\theta > \pi/5$ the contribution from $G_{11}^{(0)}$ dominates G_{11} and consequently also the scattering rate Γ_{11} . However, for the conduction electrons in the $n=2$ subband, $G_{11}^{(0)}$ has a quite large contribution to G_{22} for all scattering angles (see the thin-dashed curves in Fig. 2). We also observe that, within RPA, $\alpha_{22}G_{22}^{(0)} > \alpha_{21}G_{11}^{(0)}$. However, in TFA, $\alpha_{22}G_{22}^{(0)} < \alpha_{21}G_{11}^{(0)}$ which leads to $G_{22} < 0$. It shows that the scattering rate in the higher subband Γ_{22} within the TFA is essentially different from that within the RPA by the fact that the contribution from $G_{11}^{(0)}$ is larger than that of $G_{22}^{(0)}$. In principle, the empty subbands can also influence the scattering potential through the dielectric function within the RPA. When we include the empty subbands in the calculation, we find that the results of G_{11} and G_{22} will not be significantly modified and the contribution coming from the occupied subbands dominates the electron transport. When more than two subbands are occupied, the intersubband coupling becomes more complicated. Similarly to the two subband case, such a coupling dominates the scattering rate in higher subbands. In addition, intersubband scattering appears.

In order to test the validity of the different approximations for the screening, we compare the calculated quantum mobility with the experimental results in the Si δ -doped GaAs obtained from Shubnikov-de Haas (SdH) measurement as shown in Table I. The thickness of the doping layer in the sample is less than 20 Å. The background acceptor

concentration is 10^{14} cm^{-3} . Sample W807 was designed for a two-populated-subband system. For sample W831 and W293, there are three populated subbands. However, we could not obtain an accurate quantum mobility of the $n=3$ subband in sample W831 because of the small electron population in this subband. In the calculation, we considered the Si δ -doped GaAs with a doping layer of thickness 10 Å. It is seen that the calculated quantum mobility within the RPA is in good agreement with the experimental results. The difference between the theoretical and experimental results for all the three subbands is less than 20%. Furthermore, we also notice that the calculated mobility is larger than that from experiment. However, the mobilities within the TFA for electrons in higher subbands are substantially different from the experimental results and strongly dependent on the number of occupied subbands, which indicates the importance of including screening in the full q dependence of the dielectric matrix.⁶ The quantum mobilities within the DRPA decrease with increasing n . We conclude that the calculation within the full RPA yields electron quantum mobilities which are in agreement with the experimental results obtained from the SdH measurements for all the three subbands. This is a direct evidence of the importance of intersubband coupling effects on the ionized impurity scattering in multisubband transport. In Ref. 21 the electron mobility in δ layers was calculated by using another version of the TFA which was an extension of the TFA defined in the quantum-limit case to the multisubband system. Then the intersubband coupling is not considered and consequently the screening is the same for the electrons in the different subbands. We also calculated the quantum mobility by using this approximation and obtained almost the same values for the first three subbands.

Our calculation within the RPA shows that, in general, the subband quantum mobility in δ -doped systems decreases with increasing total electron density (the donor concentration). However, the calculated mobility indicates that, at the onset of the population of the $n=3$ and 4 subbands, the quantum mobilities μ_2^q and μ_3^q , respectively, increase very quickly to a local maximum and then decrease (also see Fig. 2(a) in Ref. 24). Such an increase in the quantum mobility is a consequence of the enhanced screening resulting from the intersubband coupling when a higher subband becomes populated. At present there is no clear indication of this effect in the experimental results. This may be due to the fact that:

- (i) it is a small effect;
- (ii) effects due to level broadening smears out such a small increase in the quantum mobility which was not considered in our calculation;
- (iii) uncertainty in the quantum mobility data of the SdH measurement is about 10%; and
- (iv) the experimental results at different densities are obtained from different samples, which may introduce fluctuations in the donor density.

Equation (10) indicates that the intersubband coupling should be more pronounced in a system in which $G_{nn}^{(0)}$ are close to each other for different n . This can be realized in a δ -doped layer placed in a quantum well (QW). Figure 3

FIG. 3. The electron density dependence of (a) the quantum mobility and (b) the transport mobility in a Si δ -doped GaAs/Ga_{0.7}Al_{0.3}As quantum well with width $W_{\text{QW}}=100$ Å (dashed curves) and 200 Å (solid curves).

shows the quantum and transport mobilities of the first two subbands in Si δ -doped GaAs/Ga_{0.7}Al_{0.3}As QW with well widths $W_{\text{QW}}=100$ Å (dashed curves) and 200 Å (solid curves). We assumed a doping layer with thickness $W_D=10$ Å which is placed in the center of the QW. It is seen that the intersubband coupling effect is much more pronounced in such a system at the onset of the occupation of a higher subband. For the 100 Å QW, the $n=2$ subband starts to be occupied at densities $N_e=3.30 \times 10^{12} \text{ cm}^{-2}$, while for the 200 Å QW, the $n=2$ and 3 subbands become populated at $N_e=1.20$ and $5.52 \times 10^{12} \text{ cm}^{-2}$, respectively. We found that, due to the occupation of the $n=2$ and 3 subbands, the quantum mobility μ_1^q and μ_2^q in the δ -doped QW are enhanced by about 50% with respect to the values before the occupation of these subbands; however, such an effect is not so pronounced in the transport mobility which is determined

by larger angle (large q) scattering. This is due to the fact that the enhancement of the screening is only significant for small q scattering.

In Fig. 4 the intrasubband scattering rate Γ_{11} for the conduction electrons in the lowest subband is depicted as a function of the scattering angle around the onset of the occupation of the $n=2$ subband in the δ -doped QW of width $W_{\text{QW}}=200$ Å. We see that, due to the occupation of the $n=2$ subband, the intersubband coupling leads to a strong screening of the small angle scattering in Γ_{11} . A kink appears in the curve of Γ_{11} vs θ when the second subband is occupied whose position corresponds to $q=2k_{F2}$. For $q \leq 2k_{F2}$, Γ_{11} is reduced considerably. Therefore, the transport mobility, dominated by the large angle scattering, does not increase appreciably at the onset of the occupation of the higher subband. We also notice that, in Fig. 3(b), μ_1^t decreases abruptly at the onset of the occupation of the $n=3$ subband in the 200 Å QW due to the intersubband scattering; but, the corresponding quantum mobility in Fig. 3(a) does not show such a change. Obviously, the change in the quantum mobility is not only dominated by the intersubband scattering but also by the screening effect resulting from the intersubband coupling which is significant for small q scattering.

In summary, we have studied the screening of the 2DEG on the ionized impurity scattering in a multisubband system. We showed that the intersubband coupling of the 2DEG plays an essential role in describing the screening properties and the ionized impurity scattering mechanism in a multisubband system. By comparing the theoretical and the experimental results of the quantum mobility in a Si δ -doped GaAs, we found that the results of the calculated mobilities when the screening is described within the RPA are in good agreement with the experimental results. Furthermore, we showed that, at the onset of the occupation of a higher subband, the change of the mobility is not only determined by the intersubband scattering but also by the intersubband coupling in the screening. The latter leads to a reduction of the small q scattering in the lower subband. We found that such an effect is significant in a δ -doped quantum well and results in a pronounced increase of the quantum mobility at the onset of the occupation of a higher subband.

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FIG. 4. The intrasubband scattering rate as a function of scattering angle for electrons in the lowest subband in a Si δ -doped GaAs/Ga_{0.7}Al_{0.3}As quantum well of width $W_{\text{QW}}=200$ Å for different electron densities: (a) 1.19; (b) 1.21; (c) 1.23; (d) 1.25; (e) 1.30; and (f) $1.40 \times 10^{12} \text{ cm}^{-2}$.

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