The influence of the surface roughness on dielectric function of two-dimensional electron gas

A Lindhard model approach

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Abstract Low field response function calculations have been performed on a two-dimensional electron gas with well-defined electron-surface roughness scattering. The Lindhard model was employed to compute the response function. In particular, detailed investigations were made on the system searching for an interplay between surface roughness with well-defined correlation function, (characterized by asperity height and correlation length) spatial confinement and the dielectric function. We analyze to what extent the normal behavior and functionality of dielectric function of two-dimensional devices are modified by random scattering events caused by the contribution from the surface roughness. Results of the current work indicate that contribution of the surface roughness on scattering and absorption process could not be considered as an underestimating effect. We find, however, that functionality of the dielectric function seems to be quite independent of the particular roughness features.

Keywords dielectric function · Surface roughness · Lindhard model

1 Introduction

Physics of low-dimensional systems has become an intense research field in the last decades. Advances in material fabrication, submicrometer technology and ultrathin film manufacturing have opened a new field in understanding the physical processes. Considering the remarkable progress in empirical manufacturing of low-dimensional systems and nano-structures and very high applications of this type

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of systems in electronic and optical devices, a vast area has been developed for physics of low-dimensional systems and nano-structure. Meanwhile some important physical effects, such as quantum Hall effect, shows that this research field could be very rich for fundamental studies [1,2,3,4,5,6,7,8].

The low-dimensional objects can be utilized as components of the electronic devices. These low-dimensional structures can provide new functionalities for new generation of electronic devices. In addition to the applicable aspects, these systems could be considered an accurate test for quantum mechanical properties. Such structures were first grown using molecular beam epitaxy (MBE) technique [9], meanwhile various techniques have been recently developed for low-dimensional system fabrication.

Today, non-homogeneous low-dimensional structures might be grown from any substance at interfaces. These structures form the basis of quantum well devices. In these structures, electron wave vector is quantized along the confining electric field. Certain experiments have shown that the quantization of the vertical component of wave vector really happens [10]. In an experiment, it was discovered by measuring optical absorption in a multi-quantum well (MQW) that absorption rate increased in specific wavelengths. These results demonstrated that vertical wave vector is quantized and empirical characteristics of absorption can be explained by step-like density of states of two-dimensional electron gas.

Due to the unavoidable surface roughness of any low dimensional system, it is essential to understand the influence of boundary scattering in physical phenomena. Formation of transverse modes, quantization of electron momentum in the systems with reduced dimensions include some aspects of physics in which surface roughness can effectively modify the optical response and electronic transport of the system. Some of the effects caused by roughness of quantum wells on electronic features have been formerly calculated [11].

In the current work, this was done about electron-photon interaction and optical features by considering successful models for the roughness. Calculations have been performed for confined electrons in a two-dimensional rough plane by introducing an appropriate correlation function for the roughness.

2 Theory and approach

We have assumed an electronic two-dimensional system in which the carriers have been confined in $x$-$y$ plane of an area $L_x \times L_y = S$. This type of structures can be realized by a semiconductor quantum well. The system has been assumed to be subjected to an external field characterizes by a vector potential, $A(r)$. This system can be described by the following Hamiltonian

$$\hat{H} = \frac{1}{2m}(\mathbf{P} - \frac{e}{c}\mathbf{A})^2 + V_{\text{conf}}(z) + \Delta V_r(r),$$

(1)

where $\mathbf{P}$ is the momentum operator, $V_{\text{conf}}(z)$ is the confining electric potential along the $z$ axis, $\Delta V_r$ is the potential introduced by roughness and $m$ is the electron mass. Then the Hamiltonian of the system in the Coulomb gauge, $\partial_i A_i = 0$, reads

$$\hat{H} = \frac{\mathbf{P}^2}{2m} + V_{\text{conf}}(z) - \frac{e}{2mc}\mathbf{A} \cdot \mathbf{P} + \frac{e^2}{2mc^2} \mathbf{A}^2 + \Delta V_r(r),$$

(2)
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The vector potential is given as follows

\[ \mathbf{A}(\mathbf{r}, t) = A_0 \hat{e} e^{i(q \cdot \mathbf{r} - \omega t)} + c.c, \]
\[ H_{ep} = \frac{eA_0}{mc} \hat{e} \cdot \mathbf{P} + \frac{eA_0}{mc} e^{-i(q \cdot \mathbf{r} - \omega t)} \hat{e} \cdot \mathbf{P}, \tag{3} \]

in which \( \hat{e} \) is the polarization vector and \( A_0 \) denotes the amplitude of the vector potential associated with an external electromagnetic field.

For this two-dimensional electron gas (2DEG) system in \( x-y \) plane, we can assume an average thickness \( L_z \) with a random rough boundary at \( z = L_z \) \( \hat{e} \) (4)

\[ z = 0, \quad z = L_z + \Delta(r), \]

where the roughness of the system characterizes by \( \Delta(r) \) which denotes deviation from the perfect two-dimensional plane at \( \mathbf{r} = xi + yj \).

If we choose the simple quantum box transverse modes in \( z \) direction given by

\[ E_{n_z} = \frac{\hbar^2 \pi n_z}{2mL_z^2}, \]

the eigenvalues of the \( H_0 = \mathbf{P}^2/(2m) + V_{conf}(z) \) can be written as \( E_{kn} = E_{n_z} + \hbar^2 k^2/(2m) \). Keeping only terms up to linear in \( A \) we arrive at the following Hamiltonian

\[ H = H_0 - \frac{e}{2mc} \mathbf{A} \cdot \mathbf{P} + \Delta V_r(r) \]
\[ = H_0 + H_{ep} + \Delta V_r(r), \tag{5} \]
\[ \Delta V_r(r) = E_{n_z}(L_z + \Delta(r)) - E_{n_z}(L_z) \]
\[ \simeq E_{n_z}(L_z) \frac{2\Delta(r)}{L_z} \tag{7} \]

Regarding the fact that \( \Delta(r) \) has been assigned randomly, this deviation should satisfy the requirement \( <\Delta(r)> = 0 \) which results in \( <\Delta V_r(r)> = 0 \) in which \( <...> \) denotes the spatial average of a typical quantity.

Gaussian type correlation functions are generally employed for roughness fluctuations. Meanwhile, the exponential correlation functions lead to a better fit with experimental results [12,13]. Due to this fact an exponential correlation function, has been employed as follows

\[ \langle \Delta V_r(r) \Delta V_r(r') \rangle = E_{n_z} \frac{4}{L_z^2} \Delta^2(r) \]
\[ = E_{n_z} \frac{4}{L_z^2} \Delta^2 \exp \left[ -|r-r'|/A \right]. \tag{8} \]

In the presence of the above mentioned relaxation mechanisms i.e. the external field and the surface roughness total scattering rate in the system is given by

\[ W(q, \omega) = \frac{4\pi}{\hbar} \sum_{i,j} |\langle \psi_i | (-e/(2mc)\mathbf{A} \cdot \mathbf{P} + \Delta V_r(r)) \psi_j \rangle|^2 \]
\[ \times \delta(E_j - E_i - \hbar \omega) |f(E_i) - f(E_j)|, \tag{9} \]
where $|\psi_i\rangle$ is the eigen-state of the unperturbed Hamiltonian, $H_0$, and $f(E)$ is the Fermi-Dirac distribution function.

The matrix elements of the relaxation couplings can be easily find to be

$$|H_{ep,kn} + \Delta V_{r,kn}|^2 = |H_{ep,kn}|^2 + |\Delta V_{r,kn}|^2 + 2\text{Re}(H_{ep,kn})^* \times \Delta V_{r,kn}.$$ (10)

The third term of the above expression could be neglected since

$$\left|\langle kn_2 | \Delta V_r(r) | k' n' 2 \rangle\right| \approx \left|\langle kn_2 | \Delta V_r(r) | k' n' 2 \rangle\right| = 0.$$ (11)

In which $\Delta V_r(r) = < \Delta V_r(r) >$. Meanwhile the second term, $| \langle kn_2 | \Delta V_r(r) | k' n' 2 \rangle|^2 = | \Delta V_{r,kn}|^2$ can be approximated as

$$| \Delta V_{r,kn}|^2 = \frac{\delta_{n_1,n'_1}}{S} \int \int e^{-i(k-k')(r-r')} \Delta V_r(r) \Delta V_r(r') d^2 r d^2 r' \approx \frac{\delta_{n_1,n'_1}}{S} \int \int e^{-i(k-k')(r-r')} (\Delta V_r(r) \Delta V_r(r')) d^2 r d^2 r'$$

$$= \frac{4}{L^2} E_{n_1}^2 \Delta_0^2 \frac{2\pi A^2}{(1 + q^2 A^2)^2} \delta_{n_1,n'_1}.$$ (12)

Accordingly the transition rate can be decomposed as

$$W(q, \omega) = W_1(q, \omega) + W_2(q, \omega),$$ (13)

in which

$$W_1(q, \omega) = \frac{2\pi}{\hbar} \left( \frac{e A_0}{mc} \right)^2 \sum_{kn_2,k' n' 2} \left| \langle kn_2 | e^{iq \cdot r} e \cdot P | k' n' 2 \rangle \right|^2 \times \delta(E_{k'} - E_k - \hbar \omega) [f(E_k) - f(E_{k'})]$$ (14)

and

$$W_2(q, \omega) = \frac{2\pi}{\hbar} \sum_{kn_2,k' n' 2} \left| \langle kn_2 | \Delta V_r(r) | k' n' 2 \rangle \right|^2 \times \delta(E_{k'} - E_k - \hbar \omega) [f(E_k) - f(E_{k'})].$$ (15)

Therefore the contribution of the surface roughness in the dielectric function is determined by $W_2(q, \omega)$. If we assume $\hat{c} = \hat{x}$ then

$$\langle kn_2 | e^{iq \cdot r} P_x | k' n' 2 \rangle = \hbar \delta_{n_1,n'_1} \delta(k' + q - k).$$ (16)

The real part of the conductivity is in the framework of the Lindhard approach is then given by

$$\sigma_{re}(q, \omega) = \frac{e^2}{2V} \frac{\hbar \omega W(q, \omega)}{\omega^2 A_0^2}.$$ (17)
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The imaginary part of the dielectric function as a function of the photon energy at different correlation lengths.

The imaginary dielectric function is given by

\[
\epsilon_{im}(q, \omega) = \frac{4\pi}{\omega} \sigma_1(q, \omega)
\]

\[
= \frac{\Gamma S}{(\hbar \omega)^2} \left[ W_1 + 2\pi \left( \frac{E_1 \Delta_0 A}{L_2 S} \right)^2 \frac{W_2}{\gamma} \right].
\]

In which \(\Gamma = e^2/(E_2^2 \pi^2)\) and \(\gamma = e^2 A_0^2/(2mc^2)\). These relations (Equations (17)-(19)) indicate that all of the mechanisms which contribute to the conductivity of the system can contribute in the amount of the dielectric function as well.

Similarly the real part of the dielectric function is given by the Kramers-Kronig relation

\[
\epsilon_{re}(q, \omega) = 1 + \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{\epsilon_{im}(q, \omega')}{\omega' - \omega} d\omega'.
\]

3 Result and Discussion

As mentioned in the previous section we have employed Lindhard model to formulate the influence of the surface roughness on the dielectric function of a two dimensional electron gas. Results of the current work have summarized in the following figures.

As depicted in Figure 1 by increasing the correlation length of the surface roughness the imaginary part of the dielectric function increases. Mean while increment of the correlation function preserves the typical functionality of the imaginary dielectric function.

Numerical results show a similar effect for the real part of the dielectric function as shown in Figure 2. This can be inferred by analyzing the physical meaning of the correlation function. The effective potential of a single local roughness, varies in spatial scale characterizes by the correlation length in the real space. High correlation length corresponds to relatively smooth systems when \(\Delta/A \ll 1\). In this
case the local rough domains have a considerable overlap. Increasing the correlation length, decreases the scattering potential of the roughness as given in Equation 12. Therefore it seems that by increasing the correlation length the imaginary part of the dielectric function (which measures the optical absorption) should be decreased ($\lim_{\Lambda \to \infty} W_2 = 0$), however it should be noted that the $W_2$ is not a monotonic function of $\Lambda$. In fact $W_2$ can be increased by increasing the $\Lambda$ when $0 < \Lambda < \sqrt{2}/q$ and decreases when $\sqrt{2}/q < \Lambda$.

Meanwhile the energy conservation rule, where enforced by the Dirac delta (Equation 15) function, finally determines the transferred momentum, $q$, and therefore the scattering rate and the effective contribution of the surface roughness in the absorption process. Since the transferred momentum during a single scattering process is limited to the range of $q < k_f$ therefore overall scattering rate increases by increasing the correlation length of the surface roughness. In this limit of the transferred momentum the scattering rate, could be increased by increasing the correlation length. Therefore the imaginary part of the dielectric function which measures the optical absorption increases by increasing the correlation length. This fact will be reflected on real part of the dielectric function, as well this fact was traced back to the Kramers, Kronig relations. It should be noted that the functionality of the real part dielectric function is not influenced by increasing the correlation length however the value of the real dielectric function effectively changes up to several order of magnitudes (Figure 2).

Accordingly since the functionality of the real part of the dielectric function will be preserved, therefore it seems that plasmon modes of the system could not significantly be affected by the magnitude of the correlation length. Meanwhile the
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Fig. 3 Imaginary part of the dielectric function as a function of the photon energy at different asperity heights.

screening length of the local charged impurities and Friedel oscillations could be influenced by the roughness parameters. Scattering rate of the system increases by increasing the asperity height and this increment is independent of the range of momentum transfer. In this case scattering rate is a monotonic increasing function of the asperity height. Therefore as reasonably expected, imaginary part of the dielectric function increases by increasing the asperity height (Figure 3).

4 Conclusion

In present work we have shown that the surface roughness significantly contributes on scattering and absorption process and dielectric function. Dielectric function of the system increases by both asperity height and correlation length of the roughness.

References

1. R. E. Prange and S. M. Girvin, The Quantum Hall Effect Springer, New York (1987)
2. R. Landauer, IBM J. Res. Dev. 1, 233 (1957)
3. M. Büttiker, Phys. Rev. Lett. 57, 1761 (1986)
4. Hong-Kang Zhao and Jian Wang, Eur. Phys. J. B 44, 93100 (2005)
5. Y.Z. He and C.G. Bao, Eur. Phys. J. B 62, 465470 (2008)
6. K. J. Thomas, J. T. Nicholls, M. Pepper, W. R. Tribe, M. Y. Simmons, and D. A. Ritchie, Phys. Rev. B 61, R13365 (2000)
7. A. A. Starikov, I. I. Yakimenko, and K.-F. Berggren, Phys. Rev. B 67, 235319 (2003)
8. N. T. Bagraev, I. A. Shelykh, V. K. Ivanov, and L. E. Klyachkin, Phys. Rev. B 70, 155315 (2004)
9. Smith, S, Chiu, L. C, Margalit, S, Yariva, A, Cho, A. Y, Infrared phys, 23, 93 (1983)
10. Grondin, R. O, Porod, W, Ho, J, Ferry, D. K, Iafrate, G. J, Superlattices Microstruct, 1, 183 (1985)
11. B. R, Nag, Semicond. Si. Tecnol. 19, 162-166 (2004)
12. A. E. Meyerovich, I. V. Ponomarev Phys. Rev B, 65, 155413 (2002)
13. S. M. Goodnick, D. K, Ferry, C. W, Wilmsen, Z. Liliental, D. Fathy, and O. L, Krivanek, Phys. Rev. B 32, 8171 (1985)
14. G. Grosso and G.P. Parravicini, Solid State Physics 255 Academic Press, London (2005)