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SCATTERING MECHANISMS FROM ROUGHNESS-INDUCED FLUCTUATIONS IN CHARGE DISTRIBUTIONS IN ZnO SURFACE QUANTUM WELLS

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Abstract. *We present a theoretical study of roughness-related scattering mechanisms for electrons in single heterostructures, especilaly in Gaussian-doped ZnO surface quantum wells. We show that besides the conventional scatterings there must exist roughness-related mechanisms of charge origin, which stem from fluctuations the electron density and the donor density in the bulk ZnO. The strength of the two charge-origin scattering sources is found to be comparable with the one of the standard one from fluctuations in the barrier position. The effect of the dielectric discontinuity on the scattering mechanisms is discussed.*

I. INTRODUCTION

Recently, zinc oxide (ZnO) has received great attention due to its potential applications in ultraviolet and blue optoelectronic devices and its unique physical properties [1, 2]. The electrical properties of heterostructures have been investigated for a long time since mobility is considered to be the *figure of merit* for material characterization. It was reported [3] that undoped thin ZnO layers shows an electron mobility of ~ 100 cm^2/Vs, lower than that of high-quality bulk ZnO. This implies that there must exits scattering mechanisms which are less relevant for bulk ZnO, but important for ZnO layers. Recently, there have been several experimental studies of transport properties of ZnO-based heterostructures [3, 4].

As known, [5] roughness-related scatterings are a key mechanism limiting mobility of heterostructures, e.g., quantum wells and heterojunctions, especially at low temperatures. Earlier theoretical investigations revealed that there exist various scattering sources related to roughness. The first-studied mechanism is due to fluctuations in the barrier position or, equivalently, local energy levels [6]. In the literature, this uncharge scattering is known simply as roughness one. Later on, one found out other roughness-related scatterings, which are charge scattering, viz., fluctuations in the electron density distribution and dipole moments at the deformed interface, which are connected with bulk charges [7] and image potential [8]. Recent experimental investigations provided evidence for the

poor quality of the ZnO surface [9, 10, 11] so that roughness-related scattering is of more importance. In Ref. [12] we showed that this dominates the electron mobility of ZnO SFQWs.

It is clear that the Coulomb repulsion between charged donors along the quantization direction gives rise to an inhomogeneous doping profile. For ion-implanted ZnO, the theoretical [13, 14] and experimental [15, 16] studies stipulate a Gaussian distribution for the impurities. This exhibits a strong dependence on coordinates. Therefore, the roughness leads to fluctuations in Gaussian impurity distribution, which must be large in comparision to those in the doping profiles explored extensively so far, where the impurity density is constant in the whole doping region. These act on 2DEG in ZnO SFQW as an important scattering source.

Thus, the aim of this paper is to present a theoretical study of scattering mechanisms in Gaussian-doped ZnO SFQWs, which originate from the roughness at the actual ZnO surface. In particular, we assess the scattering mechanisms for electrons from fluctuations in the bulk density of spatial charges and in the sheet density of charges on the deformed surface. For illustration of the theory, we calculate the carrier-density dependence of the 2DEG mobility in ZnO SFQWs.

II. GAUSSIAN-DOPED SURFACE QUANTUM WELL

II.1. Charge distributions in Gaussian-doped ZnO SFQWs

In this paper, we are concerned with single heterostructures. As a prototype, we examine the ZnO SFQW. In the system there exist charge distributions in the ZnO layer. The 2DEG is formed by, e.g., bombardement of the ZnO surface by H-ions. They are located near the ZnO surface as a strong accumulation layer, whose ditribution is given by

$$n(z) = n_s|\zeta^2(z)|, \tag{1}$$

where n_s is the electron sheet density, and $\zeta(z)$ is the envelop wave function. The 2DEG in the lowest subband is described by a standard Fang-Howard wave function [5]

$$\zeta(z) = (k^3/2)^{1/2} z e^{-kz/2} \tag{2}$$

in ZnO ($z \geq 0$) and equal to zero in the vacuum ($z < 0$). Here, k is the wave number given by a variational calculation in Ref. [12].

It was pointed out [13, 14, 15, 16] that the donor density distribution in ZnO, especially under hydrogen-ion bombardment, is of Gaussian shape with a peak at some point $z_D > 0$, so that

$$N_D(z) = \frac{n_D}{\sigma\sqrt{2\pi}} \exp\left[-\left(\frac{z - z_D}{\sigma\sqrt{2}}\right)^2\right], \tag{3}$$

in ZnO and equal to zero in the vacuum. Here, σ is a standard deviation of the Gaussian function, and the δ-doping is its limiting case with $\sigma = 0$ [17].

II.2. Low-temperature electron mobility

We are now dealing with quantum transport of electrons in ZnO SFQWs. The particles moving in the x-y plane are scattered by some disorder source, which is characterized by a random field. As known, [5] scattering by a Gaussian field is specified by its autocorrelation function in wave vector space, $\langle|U(\mathbf{q})|^2\rangle_c$. Here, the angular brackets with subindex c stand for the configuration averaging. $U(\mathbf{q})$ is a 2D Fourier transform of the unscreened scattering potential weighted with the wave function from Eq. (2),

$$U(\mathbf{q}) = \langle U(\mathbf{q},\mathbf{z})\rangle = \int dz|\zeta(z)|^2 U(\mathbf{q},\mathbf{z}). \tag{4}$$

Within the linear transport theory, the inverse transport lifetime is represented in terms of the autocorrelation function by [18]

$$\frac{1}{\tau} = \frac{1}{2\pi\hbar E_F}\int_0^{2k_F} dq \frac{q^2}{(4k_F^2 - q^2)^{1/2}} \frac{\langle|U(\mathbf{q})|^2\rangle_c}{\varepsilon^2(q)}, \tag{5}$$

where $q = 2k_F \sin(\vartheta/2)$ as the 2D momentum transfer by a scattering event in the x-y plane, with ϑ as a scattering angle. The Fermi energy is given by $E_F = \hbar^2 k_F^2/2m^*$, with $k_F = \sqrt{2\pi n_s}$ as the Fermi wave number.

The electrons in realistic ZnO SFQWs are expected to feel the following scattering sources that originate from roughness-induced fluctuations in: (i) barrier position (SR), (ii) charge distributions such as electron density (ED) and donor density (DD). The overall scattering potential (effective scattering potential-ESR) is determined by a sum of the partial ones such that

$$U_{\rm ESR} = U_{\rm SR} + U_{\rm ED} + U_{\rm DD}. \tag{6}$$

III. AUTOCORRELATION FUNCTIONS FOR ROUGHNESS-INDUCED SCATTERINGS

III.1. Fluctuation in potential barrier position

In the literature, scattering from roughness-induced fluctuations in the barrier position is most studied. The roughness causes a non-uniform shift of the barrier position from $z_b = 0$ to a local value $z_b = \Delta(\mathbf{r})$. The weighted Fourier transform of the SR potential is determined by [12]

$$U_{\rm SR}(\mathbf{q}) = F_{\rm SR}(t)\Delta_{\mathbf{q}}, \tag{7}$$

where the form factor $F_{\rm SR}$ is given in terms of the expectation values of the electric fields created by the partial confining sources. These expectations are supplied by analytic expressions derived in Ref. [12], with $\Delta_{\mathbf{q}}$ as a Fourier transform of the roughness.

III.2. Fluctuations in charge densities

III.2.1. *Electron density*

It is well known [5] that the roughness at an interface of a heterostructure also causes a non-uniform shift of charge density distributions in the system. For instance, we

consider the spatial distribution of some charged particles with a bulk density $N(z)$ in the channel layer. Its roughness-induced change is defined as

$$N\big[z-\Delta(\mathbf{r})\big]-N(z)=-\Delta(\mathbf{r})\frac{\partial N(z)}{\partial z}. \tag{8}$$

It is clear that this is subjected to fluctuations with the local roughness $\Delta(\mathbf{r})$ and, hence, acts on electrons in the channel as a scattering source. The 2D Fourier transform of the potential due to the fluctuating density is given by [5]

$$U_{\mathrm{ED}}(\mathbf{q},z)=\frac{2\pi e e_s}{\varepsilon_c q}\Delta_{\mathbf{q}}\int_0^\infty dz'\frac{\partial N(z')}{\partial z'}\Big[e^{-q|z-z'|}+\,d_\varepsilon e^{-q(z+z')}\Big], \tag{9}$$

with e_s as the charge of a particle in this density causing scattering. Here, the discontinuity in dielectric constant across the interface between the channel (ε_c) and barrier (ε_b) layers is taken into acount and is quantified by

$$d_\varepsilon=\frac{\varepsilon_c-\varepsilon_b}{\varepsilon_c+\varepsilon_b}. \tag{10}$$

In the case of ZnO SFQWs, ε_c is the dielectric constant of ZnO ($\varepsilon_c=8.2$) and ε_b the one of vacuum ($\varepsilon_b=1$). The first term on the right-hand side of Eq. (9) is due to charge-density fluctuations and the second one ($\propto d_\varepsilon$) to their image.

We are now dealing with fluctuations in the electron density ($e_s=-e$): $N(z)=n(z)$. Upon inserting Eqs. (1) and (2) for this distribution into Eq. (9), the integration is straightforward, giving

$$\begin{aligned}U_{\mathrm{ED}}(\mathbf{q},z)=-\frac{2\pi e^2 n_s a^3}{\varepsilon_c t}\Delta_{\mathbf{q}}\Bigg\{&\frac{t}{(t-a)^3}e^{-t\tilde z}-\frac{e^{-a\tilde z}}{(t-a)^2}\times\left(1-(t-a)\tilde z+\frac{a}{t-a}-a\tilde z+\frac{a(t-a)}{2}\tilde z^2\right)\\&+\frac{e^{-a\tilde z}}{(t+a)^2}\times\left(1+(t+a)\tilde z-\frac{a}{t+a}-a\tilde z-\frac{a(t+a)}{2}\tilde z^2\right)\frac{d_\varepsilon t}{(t+a)^3}e^{-t\tilde z}\Bigg\}.\end{aligned} \tag{11}$$

Hereafter, with $\sigma\sqrt{2}$ as a "natural" length unit for the above Gaussian-doped system, we introduce the dimensionless variables:

$$a=k\sigma\sqrt{2},\quad t=q\sigma\sqrt{2},\quad \tilde z=z/\sigma\sqrt{2}. \tag{12}$$

and

$$\delta=z_D/\sigma\sqrt{2}. \tag{13}$$

The theory is to be formulated in terms of these variables.

The averaging of the potential present in Eq. (11) is performed with the use of the wave function from Eq. (2). As a result, we obtain the weighted scattering potential from fluctuations in the electron density,

$$U_{\mathrm{ED}}(\mathbf{q})=-\frac{2\pi e^2 n_s}{\varepsilon_c}F_{\mathrm{ED}}(t)\Delta_{\mathbf{q}}, \tag{14}$$

where the form factor is given by

$$F_{\mathrm{ED}}(t)=\frac{a^6}{(t+a)^6}d_\varepsilon. \tag{15}$$

As clearly seen from Eqs. (14) and (15), the weighted potential is proportional to the dielectric discontinuity. This implies that within the ideal model of an infinite barrier for the Fang-Howard distribution, only the image of fluctuations in the electron density may give rise to scattering.

III.2.2. *Donor density*

Next, we are concerned with fluctuations in the donor density ($e_s = e$): $N(z) = N_D(z)$. Upon inserting Eq. (3) for this distribution into Eq. (9), consequently, one gets the Fourier transform for the potential due to donor-density fluctuations in the form:

$$U_{\rm DD}(\mathbf{q},z)=\frac{2\pi e^2 n_D e^{-\delta^2}}{\varepsilon_c t}\Delta_{\mathbf{q}}\Bigg\{\left(\delta-\frac{t+2\delta}{2}e^{(t+2\delta)^2/4}\right)\left(e^{-t\tilde{z}}\mathrm{erf}\left(\tilde{z}-\frac{t+2\delta}{2}\right)+\mathrm{erf}\left(\frac{t+2\delta}{2}\right)\right)$$
$$+te^{(t-2\delta)^2/4}e^{t\tilde{z}}\mathrm{erf}\left(\tilde{z}+\frac{t-2\delta}{2}\right)-\frac{e^{-t\tilde{z}}}{\sqrt{\pi}}\left(1+d_\varepsilon\chi(\frac{t-2\delta}{\sqrt{2}},\delta)\right)\Bigg\}, \quad (16)$$

where an auxiliary function is introduced:

$$\chi(x,y)=e^{x^2/4}\left[D_{-2}(x)-\sqrt{2}yD_{-1}(x)\right], \quad (17)$$

with $D_\nu(x)$ as a parabolic cylinder function [19].

The average of the potential present in Eq. (16) is taken with the wave function from Eq. (2).Here, by definition:

$$G_n(x,\alpha)=\frac{\partial^n}{\partial x^n}\left\{\frac{1}{x}\left(e^{\alpha x}\mathrm{erf}(-\alpha)+e^{x^2/4}\mathrm{erfc}\left(-\alpha+\frac{x}{2}\right)\right)\right\}, \quad (18)$$

$$J_n(x,\alpha)=\frac{\partial^n}{\partial x^n}\left\{\frac{1}{x}\left(e^{\alpha x}\mathrm{erfc}(\alpha)+e^{x^2/4}\mathrm{erfc}\left(\alpha-\frac{x}{2}\right)\right)\right\}, \quad (19)$$

with $n = 0,\ 1,\ 2, ...$ (integers).

$$\phi(x,y)=e^{-xy}\left[G_2(x,y)-2yG_1(x,y)+y^2G_0(x,y)\right] \quad (20)$$

and

$$\psi(x,y)=e^{-xy}\left[J_2(x,y)-2yJ_1(x,y)+y^2J_0(x,y)\right]. \quad (21)$$

As a result, the weighted potential for scattering from fluctuations in the donor density is derived to be

$$U_{\rm DD}(\mathbf{q})=\frac{\pi e^2 n_D}{\varepsilon_c}F_{\rm DD}(t)\Delta_{\mathbf{q}}, \quad (22)$$

where the form factor is given by

$$F_{\rm DD}(t)=\frac{a^3e^{-\delta^2}}{t}\Bigg\{\left(\delta-\frac{t+2\delta}{2}e^{(t+2\delta)^2/4}\right)\phi\left(t+a,\frac{t+2\delta}{2}\right)+\frac{2}{(t+a)^3}\mathrm{erf}\left(\frac{t+2\delta}{2}\right)$$
$$-te^{(t-2\delta)^2/4}\psi\left(t-a,\frac{t-2\delta}{2}\right)-\frac{2}{\sqrt{\pi}(t+a)^3}\left(1+d_\varepsilon\chi\left(\frac{t-2\delta}{\sqrt{2}},\delta\right)\right)\Bigg\}. \quad (23)$$

As observed from Eq. (23), the form factor in question is composed of two parts, a component proportional to the dielectric discontinuity and the other independenct thereof. This implies that in difference from the above case of electron-density fluctuations, for a Gaussian donor distribution both donor-density fluctuations and their image may cause scattering.

We now return to ESR scattering described by the potentials from Eq. (6). We may arrive at the weighted potential for ESR scattering,

$$U_{\mathrm{ESR}}(\mathbf{q}) = F_{\mathrm{ESR}}\Delta_{\mathbf{q}}, \tag{24}$$

where the form factor is given by

$$F_{\mathrm{ESR}} = F_{\mathrm{SR}} + F_{\mathrm{ED}} + F_{\mathrm{DD}}. \tag{25}$$

IV. RESULTS AND DISCUSSIONS

For numerical calculation, we employ the material parameters listed in Ref. [12]. With the surface roughness profile is well described a power-law distribution,

$$\langle|\Delta_{\mathbf{q}}|^2\rangle = \pi\Delta^2\Lambda^2 F_R(t). \tag{26}$$

Here, the roughness form factor is given by

$$F_{\mathrm{R}}(t) = \frac{1}{(1+\lambda^2 t^2/4n)^{n+1}}, \tag{27}$$

with n as a roughness exponent fixing its falloff at large momentum transfer t, Δ as a roughness amplitude, and Λ is a correlation length ($\lambda = \Lambda/\sigma\sqrt{2}$).
As known, ZnO (in the natural phase) has a large spontaneous polarization. For the O-polar $(000\bar{1})$ face this causes an attraction of electrons by a positive charge sheet density bound on the surface as high as 3.6×10^{13} cm^{-2}, while for the Zn-polar (0001) face a repulsion of them far away therefrom by a negative charge of the same magnitude. Thus, ESR scattering is remarkably strengthened in the former case, while weakened in the latter one.

Firstly, we deal with the roughness profile effect on the roughness scattering of the 2DEG in an O-polar face ZnO SFQW. The mobility surface roughness μ_{SR}, and effective surface roughness μ_{ESR} is plotted in Fig. 1 versus sheet electron density n_s for a fixed doping profile and various the roughness surface profile. We want to compare the roughness profile effect on scattering sources that originate from roughness induced fluctuations in: barrier position (SR), and the overall scattering potential (effective scattering potential-ESR).

Secondly, the mobility is calculated against the sheet electron density n_s for two scatterings: surface roughness μ_{SR}, and effective surface roughness μ_{ESR}. We are concerned with the roughness profile effect on ESR scattering; the comparing for the O-polar face and the Zn-polar face. The mobilities is plotted in Fig. 2(a) versus sheet electron density n_s for a fixed the doping profile and the roughness surface profile. In Fig. 2(b), the form factors for SR, ED, DD and ESR scatterings are plotted versus the dimensionless

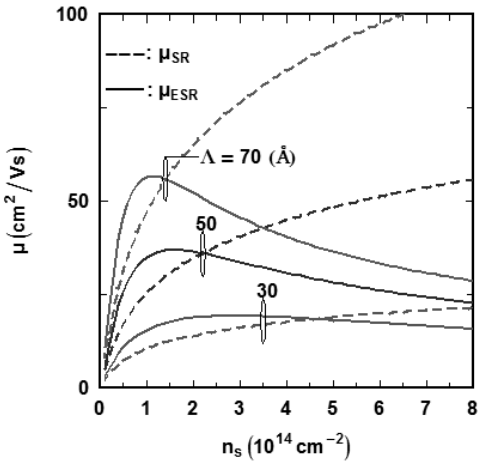

Fig. 1. Mobilities of the 2DEGs in Gaussian-doped ZnO SFQWs vs carrier density n_s for two scatterings: surface roughness (dash lines), and effective surface roughness (solid lines); the doping profile with $z_D = 6$ Å, $\sigma = 6$ Å, and various the roughness surface profile by a fixed $\Delta = 20$ Å and $n = 1$ but various the correlation lengths $\Lambda = 30$, 50, 70 Å.

momentum transfer t for a fixed sheet electron density and a doping profile.

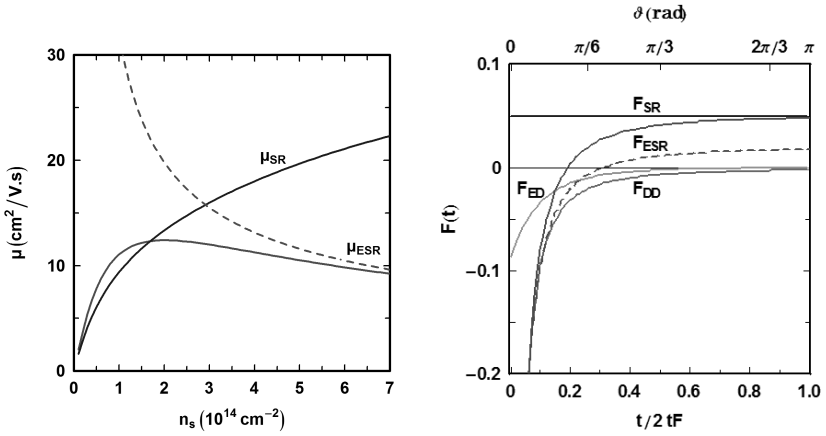

Fig. 2. (a) Mobilities of the 2DEGs in Gaussian-doped ZnO SFQWs vs carrier density n_s for two scatterings: surface roughness $\mu_{\rm SR}$, and effective surface roughness $\mu_{\rm ESR}$ with the roughness surface profile $\Delta = 30$ Å, $n = 1$ and $\Lambda = 40$ Å.(b) The form factors for SR, ED, DD, and ESR scatterings are plotted versus the dimensionless momentum transfer for a sheet electron density $n_s = 10^{14}$ cm^{-2}. Both (a) and (b) using the doping profile: $z_D = 6$ Åand $\sigma = 6$ Å. The solid lines in the O-polar face and the dashed lines in the Zn-polar one.

From the lines obtained we may draw the following conclusions.

i) As seen from Eqs. (15) and (23) both of form factors have the component proportional to the dielectric discontinuity through d_ε. The scattering rate determined by two components in Eq. (23), caused by both of the fluctuations of donor density and of their image, has more complicated behavior than one in Eq. (15) from only fluctuations of electron density.

ii) Figure 1 reveals that the calculated ESR mobility exhibits a rise with n_s up to a maximum, and then a decrease at higher n_s. On the contrary, the SR mobility shows a monotonic rise. It is connected with the role of the ED and DD scatterings for high n_s (so high n_D). Especially, this result manifest for the correlation lengths large Λ which figure 2(b) shows that the form factors $F_{\rm SR}$ and $F_{\rm DD}$ are opposite in sign ($F_{\rm DD}$ and $F_{\rm ED}$ are like in sign). As a result, the form factor $F_{\rm ESR}$ has both signs, so its absolute magnitude is smaller, but also larger than that of $F_{\rm SR}$ in dependence of the momentum transfer t (or scattering angle ϑ). At large t, $F_{\rm ESR}$ is dominated by SR scattering, so $|F_{\rm ESR}| < |F_{\rm SR}|$, however, at small t by DD scattering, so $|F_{\rm ESR}| > |F_{\rm SR}|$. As indicated [20], the angular distribution of the roughness profile from Eq. (27) is such that for very small Λ (rough interface) this is nearly isotropic, while with large Λ (smooth interface) this is concentrated at small angles.

iii) As seen from the in Fig. 2(a), for the comparison between the ESR and SR mobilities depends on the sheet electron density n_s. At $n_s < 2.1 \times 10^{14}$ cm^{-2}, one has: $\mu_{\rm ESR} > \mu_{\rm SR}$, however, at $n_s > 2.1 \times 10^{14}$ cm^{-2}: $\mu_{\rm ESR} < \mu_{\rm SR}$. This is connected with relative role of the form factors for SR, ED and DD scatterings which is revealed in Fig. 2(b). At higher n_s, where DD and ED scattering is dominant (the DD scattering is more dominant the ED one), so $|F_{\rm ESR}| > |F_{\rm SR}|$ and $\mu_{\rm ESR} < \mu_{\rm SR}$. This implies the importance of DD scattering at extremely high doping levels.

iv) The large polarization charges bound on the ZnO surface lead to a remarkable decrease the mobility of electrons confined in the O-polar face ZnO SFQW, whereas an increase in the Zn-polar face one, but the DD scattering will dominate at extremely high doping levels, so the mobility of electrons is equivalent when it is confined in the O-polar face or the Zn-polar one.

V. CONCLUSION

In this paper, we have presented a full treatment of scattering mechanisms in ZnO SFQWs which stem from surface roughness. We prove that besides the well-known sources, there exist new scatterings from fluctuations in a non-uniform distribution of charge density (ED) and those of the donor density (DD) in the bulk ZnO by the deformed ZnO surface. We hope that our analytic results stimulate theoretical investigations and help to clarify the experimental results existing as a challenge for decades. Our theory is applicable to various bilayer heterostructures.

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