# Effects of surface roughness and alloy disorder on the density of states in semiconductor quantum wires

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We calculate the effects of surface roughness and alloy disorder on the density of states (DOS) in cylindrical semiconductor quantum wires with inclusion of a Hubbard local-field correction. It is found that the disorder-induced DOS tail becomes much larger and much more extended below the subband edge when reducing the wire size. Further, the DOS tail at low energies may be enhanced by the Hubbard correction by up to several orders of magnitude. A possibility of applying our results to describe the observed inhomogeneous broadening of exciton lines in the absorption and emission spectra of quantum wires is discussed.

## I. INTRODUCTION

There has been a growing interest in semiconductor quantum wire (QWR) structures. These structures have opened up the potential for various device applications. It is well known that the density of states (DOS) is of fundamental importance in theoretical and experimental analysis of observable properties of the disordered quasi-one-dimensional electron gas (1DEG) in the wire. The disorder in QWR's is of different origins, e.g., impurity doping, surface roughness, and alloy disorder.[1]

So far, almost all of the existing theories[2–4] of disorder effects on the 1D DOS of QWR's have been focused only on the one arising from impurity doping, ignoring the other sources of disorder. The latter have recently been confirmed experimentally to be important in very thin QWR's, e.g., surface roughness in wires made from $GaAs/Al_xGa_{1-x}As$ (Refs. 5,6) and alloy disorder in wires from $In_{1-x}Ga_xAs/InP$.[7,8] Moreover, it has been shown[9] that the local-field correction due to many-body interactions in the 1DEG is to be invoked in determining the disorder effects on electronic properties of the wire, e.g., the electron mobility.

Thus, the aim of the present paper is to supply an estimate of the effects on the 1D DOS in QWR's due to surface roughness and alloy disorder with inclusion of a local-field correction.

## II. BASIC EQUATIONS

To start with, we will collect the formulas to be used for calculating the energy spectrum of disordered 1DEG's in QWR's. The disorder is normally caused by some random field affecting the motion of electrons along the wire axis. Recently, upon developing a 1D version of the path-integral approach we have proved[10] that the DOS of disordered 1DEG's over the entire energy spectrum may be obtained by matching the semiclassical and quantum components. The first component describes the DOS in the high-energy region (above and near the subband edge) and is connected with long-range fluctuations in the disorder potential. The semiclassical DOS is provided by a simple analytic expression:

$$\rho(E)=\frac{1}{\pi}\left(\frac{2m}{\hbar^2}\right)^{1/2}\frac{1}{(2\gamma)^{1/2}}\exp\left(-\frac{E^2}{4\gamma^2}\right)\times\left[D_{-1/2}\left(-\frac{E}{\gamma}\right)-\frac{\hbar^2F^2}{24m\gamma^3}D_{5/2}\left(-\frac{E}{\gamma}\right)\right], \quad (1)$$

in which $D_\nu(x)$ is a parabolic cylinder function,[11] and $m$ is the effective mass for a parabolic 1D subband: $E(k)=\hbar^2k^2/2m$. Here $\gamma$ and $F$ denote the rms of the potential and force of the random field. These are given in terms of a Fourier transform of the autocorrelation function $W(k)$ of the field in question by

$$\gamma^2=\int_{-\infty}^{\infty}\frac{dk}{2\pi}W(k) \quad (2)$$

and

$$F^2=\int_{-\infty}^{\infty}\frac{dk}{2\pi}k^2W(k). \quad (3)$$

The second component describes the DOS in the low-energy (deep-tail) region and is associated with the short-range potential fluctuations. The quantum DOS is supplied in the following analytic form:

$$\rho(E)=\frac{1}{\pi}\left(\frac{2m}{\hbar^2}\right)^{1/2}\frac{\hbar\omega}{\sqrt{2}Q_\omega^{3/2}}\exp\left[-\frac{(\hbar\omega/4-E)^2}{4Q_\omega^2}\right]\times D_{1/2}\left(\frac{\hbar\omega/4-E}{Q_\omega}\right). \quad (4)$$

Here $Q_\omega$ means a weighted rms potential and is to be defined as a function of the parameter $\omega$ in terms of the Fourier transform of the autocorrelation function by

$$Q_\omega^2=\int_{-\infty}^{\infty}\frac{dk}{2\pi}W(k)\exp\left[-\frac{E(k)}{\hbar\omega}\right]. \quad (5)$$

 

The parameter $\omega$ is the curvature of a nonlocal harmonic well modeling the autocorrelation function and is, in turn, given as a function of energy: $\omega=\omega(E)$, by a variational (transcendental) equation

$$\int_{(\hbar\omega/4-E)/Q_\omega}^{\infty} dx \exp\left(-\frac{x^2}{4}\right)\left(x-\frac{\hbar\omega/4-E}{Q_\omega}\right) \times\left\{\left[\frac{Q_\omega}{\hbar\omega/4}-6\frac{Q'_\omega}{\hbar}-x\left(1-4x\frac{Q'_\omega}{\hbar}\right)\right]D_{1/2}(x) +\frac{1}{2}\left(1-4x\frac{Q'_\omega}{\hbar}\right)D_{1/2}(x)\right\}=0, \tag{6}$$

in which $Q'_\omega=dQ_\omega/d\omega$. Thus, the function $\omega(E)$ is determined, according to Eqs. (5) and (6), by the autocorrelation function in wave-vector space, which depends both on the wire geometry and the disorder origin.[1,12]

It is clearly seen from Eqs. (1)–(6) that the autocorrelation function of a random field plays the key role as the input function for disorder interaction in our DOS calculation. To find this, we need to specify our model of QWR's by choosing a circular cylinder and confine the motion of the electrons in the cylinder by an infinite potential barrier at its surface. At zero temperature almost all electrons are assumed to occupy the lowest subband, as evidenced experimentally. Based on these assumptions of the electron system, one may deduce the autocorrelation function of interest.

Random fluctuations in the wire radius are normally assumed to be Gaussian-like. The autocorrelation function for surface roughness is then given by[1]

$$W_{\mathrm{SR}}(k)=(2.4)^4\sqrt{\pi}\frac{\hbar^4}{m^2}\frac{\Delta^2\Lambda}{R^6}\frac{\exp(-\Lambda^2k^2/4)}{\epsilon^2(k)}. \tag{7}$$

Here $R$ denotes the wire radius, $\Delta$ and $\Lambda$ are the average radius fluctuation and the correlation length along the wire axis, and $\epsilon(k)$ the static dielectric function allowing for screening the disorder interaction by 1D electrons.

Fluctuations in the composition of a semiconductor alloy can produce a strong effect, especially when the electron system and the alloy disorder are not separated in space as in the case of $In_{1-x}Ga_xAs/InP$. The autocorrelation function for alloy disorder inside a cylindrical wire is written as[12]

$$W_{\mathrm{AD}}(k)=x(1-x)\frac{2.03a^3}{4\pi R^2}\frac{(\delta V)^2}{\epsilon^2(k)}, \tag{8}$$

where $\delta V$ is the rms spatial average of the fluctuating alloy potential over the alloy unit cell, and $a^3$ is the unit cell volume. Since $\epsilon(k)\to 1$ for $k\to\infty$,[9] the average potential $\gamma$ and force $F$ related to composition fluctuations are, according to Eqs. (2), (3), and (8), divergent. Therefore, in the case of alloy disorder, the semiclassical DOS (1) is inapplicable, and the quantum DOS (4) is to be extended to higher energies.

It is well known[1,9] that screening by 1DEG's in QWR's is generally of importance in determining the disorder effects on electronic properties, e.g., the electron mobility. At zero temperature, this is quantified by a static dielectric function, defined by

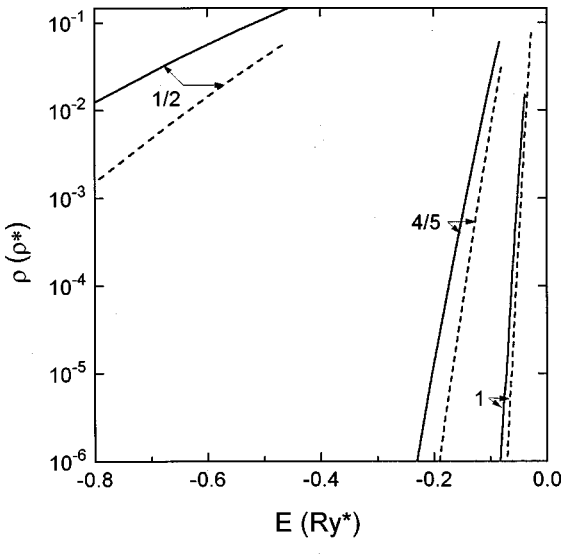


FIG. 1. Quantum DOS $\rho(E)$ vs energy for the 1DEG in a wire subjected to surface roughness with $\Delta=3$ Å, $\Lambda=60$ Å, under an electron density $n_e=5\times10^5$ cm$^{-1}$ and different wire radii $R$ (denoted on lines in units of $a^*$). The solid and dashed lines refer to screening with and without Hubbard correction, respectively.

$$\epsilon(k)=1+\frac{2m}{\pi\hbar^2}\frac{v(k)}{\mathrm{k}}[1-G(k)]\ln\left|\frac{\mathrm{k}+2k_{\mathrm{F}}}{\mathrm{k}-2k_{\mathrm{F}}}\right|, \tag{9}$$

with $\mathrm{k}=|k|$. Here $v(k)$ stands for the electron-electron interaction potential, $G(k)$ is the local-field factor, and $k_{\mathrm{F}}$ the Fermi wave vector fixed by the 1D carrier density $n_e$ via $k_{\mathrm{F}}=(\pi/2)n_e$. The electron-electron interaction is to be weighted with the lowest-subband wave function, given by[10]

$$v(k)=\frac{4e^2}{\epsilon_{\mathrm{L}}}\frac{1}{(\mathrm{k}R)^2}[1-2I_1(\mathrm{k}R)K_1(\mathrm{k}R)], \tag{10}$$

with $\epsilon_{\mathrm{L}}$ the dielectric constant of the background lattice. Here $I_1(x)$ and $K_1(x)$ are the first-order modified Bessel functions of the first and second kind.[11] The local-field factor takes into account the effects due to exchange and correlation in the 1DEG. In the random phase approximation, where these are neglected, one sets $G(k)=0$. The function $G(k)$ may be derived within the Singwi-Tosi-Land-Sjölander self-consistent scheme.[9] A simpler analytic result for the local-field factor is obtained in the Hubbard approximation,[1] where only the exchange effect is involved:

$$G(k)=\frac{1}{2}\frac{v(\sqrt{k^2+k_{\mathrm{F}}^2})}{v(k)}. \tag{11}$$

## III. RESULTS AND CONCLUSIONS

We have carried out numerical calculations for cylindrical QWR's made from $In_{1-x}Ga_xAs/InP$ ($x=0.47$). The material parameters are $m=0.041\ m_e$, $\epsilon_{\mathrm{L}}=13.3$. The results are presented in the atomic units for the length, the energy, and the 1D DOS: the effective Bohr radius $a^*=\epsilon_{\mathrm{L}}\hbar^2/me^2=172$ Å, the effective rydberg $\mathrm{Ry}^*=me^4/2\epsilon_{\mathrm{L}}^2\hbar^2=3.15$ meV, and $\rho^*=1/\mathrm{Ry}^*a^*=1.85\times10^5$ meV$^{-1}$ cm$^{-1}$, respectively.

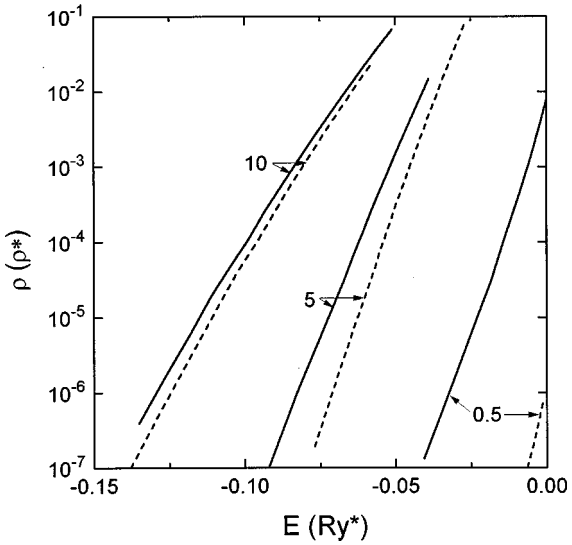


FIG. 2. The interpretation is the same as in Fig. 1 but under a wire radius $R=a^*$ and various electron densities $n_e$ (denoted on lines in units of $10^5$ cm$^{-1}$).

Figures 1 and 2 display the quantum DOS of the 1DEG in a wire subjected to surface roughness with[12] $\Delta=3$ Å, $\Lambda=60$ Å. In Fig. 1, this is plotted under an electron density $n_e=5\times10^5$ cm$^{-1}$ and different wire radii $R=a^*/2$, $4a^*/5$, $a^*$, and $2a^*$, whereas in Fig. 2 under a wire radius $R=a^*$ and various electron densities $n_e=5\times10^4$, $5\times10^5$, and $10^6$ cm$^{-1}$. The solid and dashed lines refer to screening with and without Hubbard correction, respectively. Figure 3 illustrates the matching of the two components of the function $\rho(E)$ in the presence of the surface roughness: the quantum DOS (4) for the low-energy tail (solid lines) and the semiclassical DOS (1) for the high-energy region (dashed ones). This is plotted with inclusion of Hubbard correction under an electron density $n_e=5\times10^5$ cm$^{-1}$ and different wire radii $R=a^*/5$, $a^*/4$, and $a^*/3$. Figures 4 and 5 sketch the DOS of the 1DEG subjected to alloy disorder with[12] $\delta V=0.6$ eV, $a=5.9$ Å. This is plotted in Fig. 4 (or Fig. 5) under the same conditions as in Fig. 1 (or Fig. 2).

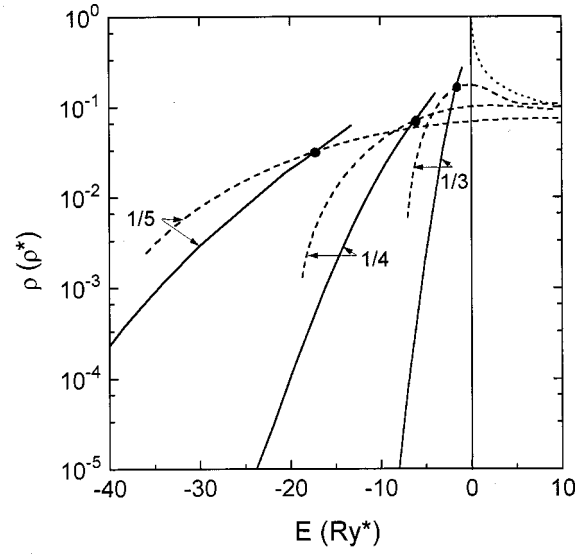


FIG. 3. Full DOS $\rho(E)$ vs energy below and above the subband edge for the 1DEG in the presence of the surface roughness under an electron density $n_e=5\times10^6$ cm$^{-1}$ and different wire radii $R$ (denoted on lines in units of $a^*$). The solid lines refer to the quantum DOS, and the dashed ones to the semiclassical DOS, their intersection points are marked by a full circle. The dotted line represents the DOS of the ideal 1DEG.

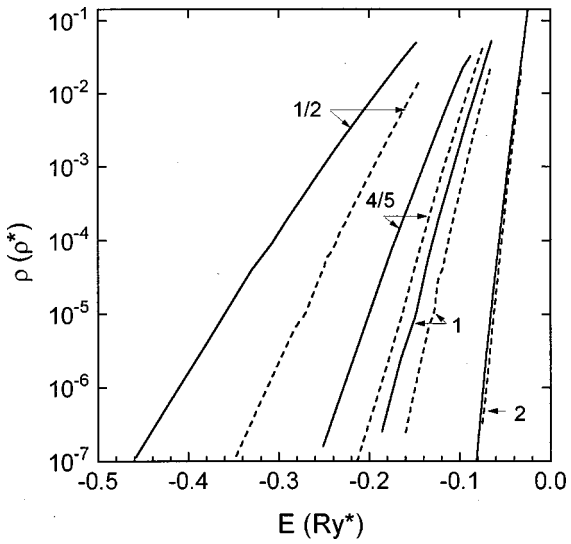


FIG. 4. Quantum DOS $\rho(E)$ vs energy for the 1DEG in a wire subjected to alloy disorder with $\delta V=0.6$ eV, $a=5.9$ Å, under an electron density $n_e=5\times10^5$ cm$^{-1}$ and different wire radii $R$ (denoted on lines in units of $a^*$). The solid and dashed lines refer to screening with and without Hubbard correction, respectively.

From the results thus obtained, we may draw the following conclusions.

(i) Figures 1–5 indicate the disorder arising from surface roughness and alloy disorder basically changes the DOS of the 1DEG in a wire, giving rise to a tail of localized states far below the subband edge.

(ii) It follows from Figs. 1, 3, and 4 that the disorder-induced DOS tail drastically depends on the wire size. In-

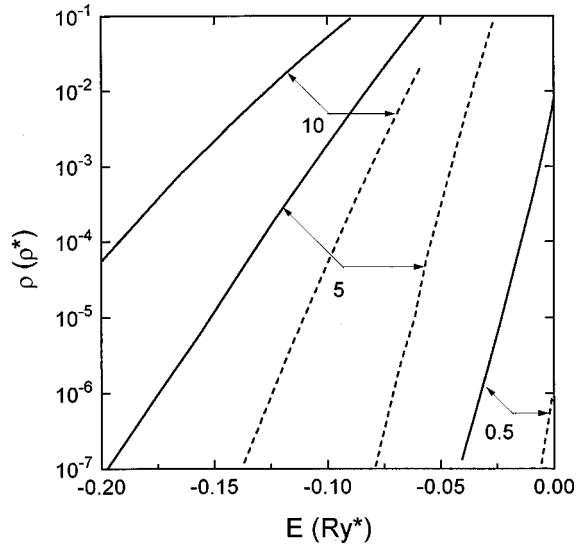


FIG. 5. The interpretation is the same as in Fig. 4 but under a wire radius $R=a^*$ and various electron densities $n_e$ (denoted on lines in units of $10^5$ cm$^{-1}$).

deed, the DOS tail becomes much larger and much more extended below the subband edge with reduction of the wire radius. This means that the thinner the wire, the stronger the disorder effect is. Figure 3 also reveals with reducing the wire radius, both the quantum and semiclassical DOS tails are more extended, so that their intersection point moves towards lower energies. An examination of Figs. 1 and 4 shows that the wire-radius dependence of the DOS tail due to surface roughness is stronger than that due to alloy disorder. For the material used, the DOS tails due to surface roughness and alloy disorder are seen to almost coincide for the wire radius $R=4a^*/5$. For $R<4a^*/5$, the surface-roughness DOS tail overwhelms the alloy-disorder one, but for $R>4a^*/5$, the latter is dominant, the former being negligible for $R=2a^*$.

(iii) A comparison of the solid and dashed lines in Figs. 1, 2, 4, and 5 indicates the Hubbard correction is of importance at low energies. This can increase the quantum DOS by up to several orders of magnitude.

(iv) It is found from Figs. 1 and 4 that the separation between relevant solid and dashed lines increases with reduction of the wire radius. This means that the thinner the wire, the more important the Hubbard correction is. The exchange effect may be ignored only for thick wires, e.g., of radius $R>2a^*$. Also, Figs. 2 and 5 show the effect is larger at a lower electron density.

To end, it is interesting to suggest that our results may be applied to describe the inhomogeneous broadening of exciton lines in the absorption and emission spectra of QWR's. It has been just recently experimentally reported[13,14] that localization of the 1D exciton is the main channel of radiative processes occurring in QWR's at low temperatures. Moreover, in order to account for fine details of the experimental findings, one should include in the analysis disorder caused by surface roughness and composition fluctuations.[15] It has been pointed out[16] that within the adiabatic approximation where the energies of electron and hole quantization (inside the wire) as well as the binding energy of the 1D exciton are large compared with the inhomogeneous broadening, the rate of radiative processes due to the 1D exciton is, crudely speaking, proportional to the density of states of its center-of-mass motion along the wire axis. Thus, the disorder-induced tail of localized states of the exciton center of mass (lying below the ground state of the ideal exciton) gives rise to the observed broadening of the exciton lines.

## ACKNOWLEDGMENTS

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