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Localization theory of surface exciton polaritons on a rough semiconductor surface

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Abstract

We develop a numerical model to investigate the localization of surface exciton polaritons in the presence of random roughness and spatial dispersion. The localization criteria are examined. The localization effects are embodied in the large enhancement and rapid decay of the field intensity on the surface. The calculation shows that there is a transition from the localized state to the extended state. It has been found that the localization occurs in a limited frequency range above the resonant frequency of transverse excitons.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In semiconductor systems with reduced dimensionality, the exciton polariton picture is greatly modified. For example, exciton states in two-dimensional semiconductor systems exhibit the effect of quantum-mechanical level repulsion [1]. In semiconductor systems of quantum dots, the exciton polariton properties are affected by the long-range radiative interaction between quantum dots [2]. It has been shown that pulsed near-field excitation in semiconductor quantum wells results in the propagation of excitonic wave packets [3]. Recently, there has been growing interest in studies of surface polaritons with the development of applied surface science [4–6]. Meanwhile, researchers have studied the localization of the surface phonon and plasmon polaritons caused by surface roughness [7–9]. Many of the ideas about the localization of electromagnetic (EM) waves have been suggested by John [10] and Anderson [11]. In the last two decades, optical experiments on randomly rough surfaces have observed a variety of qualitative and quantitative changes in phenomena that exist in the absence of the roughness [12]. Quantitative changes are very significant. A notable example is the surface-enhanced Raman scattering (by five to six orders of magnitude). Surface polaritons on randomly rough surfaces were always considered to be in an extended state. Now it has been realized that weak roughness can cause a major changing of states from extended to localized states [13, 14].

The previous theoretical and experimental studies have mainly concentrated on the localization of surface plasmon polaritons on a rough metallic surface. However, in solid state spectroscopy most devices are made of semiconductors. Wannier excitons are elementary excitations of semiconductors. The Wannier exciton is weakly bound by a hole from the valence band and an electron from the conduction band, with an electron–hole separation large in comparison with a lattice constant. A photon whose frequency is near an exciton resonance energy will couple strongly with the excitation of a semiconductor. The exciton–polariton, a mixed mode of a photon and an exciton, is the true eigenmode of EM wave propagation in the semiconductor. However, there is a forbidden band between the resonant frequencies of transverse and longitudinal excitons, in which the real part of the dielectric function of a semiconductor is negative. Therefore, EM waves with frequencies in the forbidden band cannot travel in the thick semiconductor. In this case, the EM waves can propagate as surface exciton polaritons on the semiconductor surface. The surface exciton polaritons cannot decay into photons radiating away from the surface and also they cannot be excited by simply shining light onto the flat surface of a single semiconductor, because the conservation of energy and momentum between incident photons and surface exciton polaritons is not satisfied simultaneously.

Real semiconductor surface are randomly rough to some degree, so the conservation of momentum parallel to the surface is invalid. In this case, linear optical excitation of surface exciton polaritons on a randomly rough surface of a single semiconductor becomes possible. On the other hand, the surface roughness can cause the localization of surface exciton polaritons, i.e., they cannot propagate on the surface. To study the localization of surface exciton polaritons, we require inclusion of spatial dispersion, i.e., the wavevector dependence of the dielectric function. This dependence leads to particular properties of the localization of surface exciton polaritons which differ from those of the other surface polariton localization. The detailed study of the localization of surface exciton polaritons therefore gives information about the similarities of and the differences between various surface polaritons. In the present paper, we propose the localization theory of surface exciton polaritons due to the incidence of a Gaussian beam of laser light. Our aim is to answer the following questions: (i) what are the localization criteria of surface exciton polaritons? (ii) what are the new localization effects of surface exciton polaritons? (iii) what is the dependence of the field intensity of surface exciton polaritons on localization? The answers to the above questions are fundamental to the observation of localization of surface exciton polaritons.

The remainder of this paper is organized as follows. Section 2 deals with the dispersion theory of surface exciton polaritons. Section 3 formulates the average EM field intensity outside a randomly rough surface. The localization theory of surface exciton polaritons is proposed in section 4. The numerical results on localization are presented in section 5. Section 6 gives our discussion.

2. Dispersion theory of surface exciton polaritons

For convenience the semiconductor under study is taken to be of cubic symmetry, so that it is optically isotropic. In the exciton energy region, one must consider the spatial dispersion in the dielectric response of the semiconductor. In general, the spatial dispersion of the semiconductor is described by a wavevector-dependent dielectric function $\epsilon(k, \Omega)$. For a one-band model of Wannier excitons, the dielectric function of the semiconductor is given in the form neglecting the damping [15],

$$\epsilon(k, \Omega) = \epsilon_\infty \left(1 + \frac{\omega_{\mathrm{L}}^2 - \omega_{\mathrm{T}}^2}{\omega_{\mathrm{T}}^2 + \beta k^2 - \Omega^2}\right), \tag{1}$$

where ϵ_∞ is the high-frequency dielectric constant of the semiconductor and ω_T and ω_L are the resonant frequencies of the transverse and longitudinal excitons in the semiconductor. The influence of spatial dispersion is described by $\beta = \hbar\omega_T/m^*$, where m^* is the translational effective mass of excitons and $\hbar$ is Planck's constant divided by 2π.

The exciton polariton is a mixed mode of a photon and an exciton, and it is the true eigenmode of the propagation of EM waves in the semiconductor bulk. For given wavevector **k**, there are three branches of exciton polariton waves, of which one is longitudinal (called mode L) and the other two are transverse. If the longitudinal mode in the bulk has the dielectric constant ϵ_L and the wavevector k_L, then it is the solution of the equation $\epsilon_L = \epsilon(k_L, \Omega) = 0$, which yields the dispersion relation $\Omega^2 = \omega_L^2 + \beta k_L^2$. The dispersion relation of transverse exciton polaritons has the form

$$\frac{c^2k^2}{\Omega^2} = \epsilon(k, \Omega), \tag{2}$$

where c is the vacuum velocity of light. For given frequency Ω, equation (2) is quadratic in k^2, with the solution being

$$k_{1,2}^2(\Omega) = \left\{-c^2\omega_T^2 + c^2\Omega^2 + \epsilon_\infty\beta\Omega^2 \pm \left[(c^2\omega_T^2 - c^2\Omega^2 - \epsilon_\infty\beta\Omega^2)^2 - 4c^2\beta(\epsilon_\infty\Omega^4 - \epsilon_\infty\omega_L^2\Omega^2)\right]^{\frac{1}{2}}\right\} \times (2c^2\beta)^{-1}, \tag{3}$$

where 1 and 2 refer to the plus and minus signs, respectively. Thereby one can define the dielectric functions

$$\epsilon_{1,2}(\Omega) = \frac{c^2k_{1,2}^2(\Omega)}{\Omega^2}. \tag{4}$$

On the plane of frequency versus wavevector, the first and second transverse modes are the lower and upper exciton–polariton branches with dielectric functions ϵ_1 and ϵ_2, respectively. The coexistence of three bulk modes at a given energy complicates a simple reflection experiment and its theoretical fit by Fresnel's equations. The reason is that a transverse wave incident on a spatially dispersive semiconductor in general excites all three bulk modes in the semiconductor with certain amplitudes. The two Maxwell's boundary conditions for tangential electric and magnetic fields from which Fresnel's equations are derived do not suffice to determine the amplitude ratios of the three waves inside the semiconductor. One needs additional information expressed in the form of the so-called additional boundary condition, subsequently abbreviated ABC.

Let us consider the boundary between a spatially dispersive semiconductor and the vacuum with dielectric constant $\epsilon_0 = 1$, which both fill up infinite half spaces. The z-axis is normal to the semiconductor surface and points to the vacuum. We search for the eigenstates of the surface of the semiconductor in the exciton energy region. The eigenstates of the surface are those EM waves, of which one is the transverse mode in the vacuum (called mode 0) obeying the dispersion relation $k_0 = \Omega/c$ and the other three modes belong to the two transverse exciton–polariton modes and to the longitudinal one inside the semiconductor. All these modes are matched together at the semiconductor surface by the Maxwell boundary conditions and the ABCs to form the eigenstates of the surface. We call the quanta of this eigenstate surface exciton polaritons if the mode 0 is localized at the surface and is travelling nearly parallel to it. To explore the properties of surface Wannier exciton polaritons we split the wavevectors into components parallel and perpendicular to the surface. The component **n** parallel to the surface is the same for all waves outside and inside the semiconductor because of the phase-matching condition. The components perpendicular to the surface are then given by $k_{jz}^2 = k_j^2 - \mathbf{n}^2$, where $j = 0, 1, 2, L$.

We define the electric field amplitudes $\mathbf{E}_0$ of the transverse mode 0 outside the semiconductor, and the amplitudes $\mathbf{E}_1$ and $\mathbf{E}_2$ of the transverse modes and $\mathbf{E}_\mathrm{L}$ of the longitudinal mode inside the semiconductor. The electric fields are all polarized parallel to the plane of incidence because only this geometry yields surface exciton polaritons. The conservation of the tangential component of the electric field amplitude may then be written:

$$E_0 k_{0z}/k_0 = E_1 k_{1z}/k_1 + E_2 k_{2z}/k_2 + E_\mathrm{L} n/k_\mathrm{L}. \tag{5}$$

The magnetic field is already tangential. The conservation of the tangential magnetic field amplitude yields

$$E_0 \epsilon_0/k_0 = E_1 \epsilon_1/k_1 + E_2 \epsilon_2/k_2. \tag{6}$$

Equations (5) and (6) are the two Maxwell boundary conditions of surface exciton polaritons. They connect the electric field amplitudes of one wave outside and three waves inside the semiconductor. The explicit behaviour of surface exciton polaritons depends on the ABC which connects the electric field amplitudes inside the semiconductor. Hopfield and Thomas proposed a reasonable ABC, which assumes that the excitonic contribution to the macroscopic polarization should vanish at the surface [15]. The excitonic polarizations are directly proportional to $(\epsilon_j - \epsilon_\infty)\mathbf{E}_j$, where $j = 1, 2, \mathrm{L}$. Splitting the electric field vectors into components parallel and perpendicular to the surface yields two special equations for surface exciton polaritons:

$$E_1(\epsilon_1 - \epsilon_\infty)k_{1z}/k_1 + E_2(\epsilon_2 - \epsilon_\infty)k_{2z}/k_2 - E_\mathrm{L}\epsilon_\infty n/k_\mathrm{L} = 0, \tag{7}$$

$$E_1(\epsilon_1 - \epsilon_\infty)n/k_1 + E_2(\epsilon_2 - \epsilon_\infty)n/k_2 + E_\mathrm{L}\epsilon_\infty k_{\mathrm{L}z}/k_\mathrm{L} = 0. \tag{8}$$

Equations (5)–(8) form a system of four linear equations for the four unknown electric field amplitudes E_0, E_1, E_2, and E_L. This system has a solution only if the determinant equals zero:

$$\begin{aligned}\epsilon_1(\epsilon_2 - \epsilon_\infty)(\epsilon_\infty k_{0z} - \epsilon_0 k_{1z})\mathbf{n}^2 - \epsilon_2(\epsilon_1 - \epsilon_\infty)(\epsilon_\infty k_{0z} - \epsilon_0 k_{2z})\mathbf{n}^2 + \epsilon_\infty k_{\mathrm{L}z} \\ \times [\epsilon_1(\epsilon_2 - \epsilon_\infty)k_{0z}k_{2z} - \epsilon_2(\epsilon_1 - \epsilon_\infty)k_{0z}k_{1z} + \epsilon_0(\epsilon_1 - \epsilon_2)k_{1z}k_{2z}] = 0.\end{aligned} \tag{9}$$

Equation (9) is the dispersion relation between the wavevector $\mathbf{n}$ and the frequency Ω of surface exciton polaritons for the chosen ABC.

The dispersion relation contains in general complex quantities because the wavevectors k_z may have imaginary parts. Thus, surface exciton polaritons must have complex frequency Ω even for real wavevector $\mathbf{n}$. The real part of k_{jz} determines the travelling direction of each mode j, the imaginary part the direction of the spatial decay. To give a physically meaningful solution of the dispersion relation, the wavevectors k_{jz} have to be chosen as follows [16]:

$$\begin{aligned}&\mathrm{Re}\, k_{0z} < 0 \quad \text{with } \mathrm{Im}\, k_{0z} > 0, \qquad \mathrm{Re}\, k_{1z} < 0 \quad \text{with } \mathrm{Im}\, k_{1z} > 0, \\ &\mathrm{Re}\, k_{2z} > 0 \quad \text{with } \mathrm{Im}\, k_{2z} < 0, \qquad \mathrm{Re}\, k_{\mathrm{L}z} > 0 \quad \text{with } \mathrm{Im}\, k_{\mathrm{L}z} < 0.\end{aligned} \tag{10}$$

Equation (9) has to be solved numerically to obtain the frequency versus wavevector relation of surface exciton polaritons. The energy of Wannier excitons is given by a hydrogen-like energy series with main quantum number n. We made a numerical evaluation for the $C_{n=1}$ exciton in ZnO neglecting the anisotropy of this crystal. The parameters concerned [17] are as follows: $\hbar\omega_\mathrm{T} = 3.4215$ eV, $\hbar\omega_\mathrm{L} = 3.4323$ eV, $\epsilon_\infty = 6.16$, and $m^* = 0.87 m_\mathrm{e}$, where m_e is the electron mass. Figure 1 shows the variation of the real part of the complex frequency Ω with real wavevector n. As shown, $\mathrm{Re}\,\Omega = \omega_\mathrm{T}$ at $n = \omega_\mathrm{T}/c$, $\mathrm{Re}\,\Omega$ is a monotonically increasing function of n, and $\mathrm{Re}\,\Omega$ exceeds ω_L at large wavevectors. Figure 2 shows the variation of the imaginary part of complex frequency Ω with real wavevector n. The appearance of an imaginary part is a signature that surface exciton polaritons have a decay rate due to the spatial dispersion, which is denoted by $\Gamma_\mathrm{s} = -\mathrm{Im}\,\Omega$.

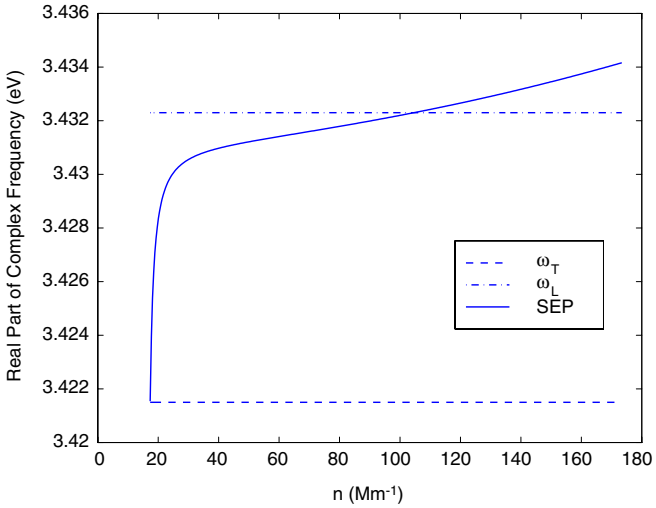

Figure 1. The dispersion relation for surface exciton polaritons (SEPs) is plotted for the real wave vector **n** parallel to the surface and the real part of complex frequency Ω. ω_T and ω_L are the resonant frequencies of transverse and longitudinal excitons.

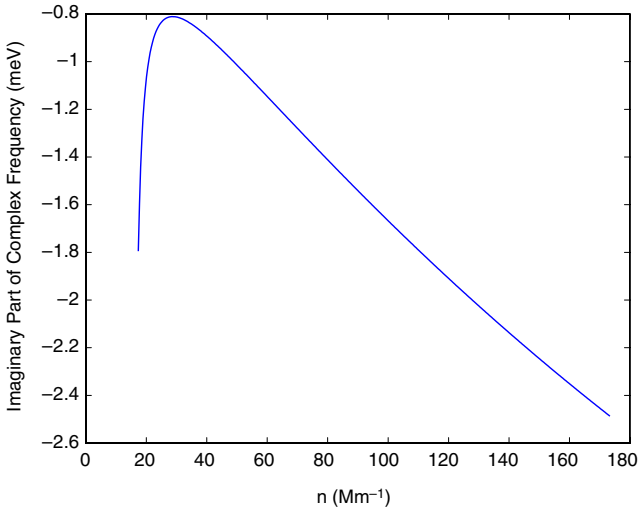

Figure 2. The dispersion relation for surface exciton polaritons is plotted for the real wavevector **n** parallel to the surface and the imaginary part of complex frequency Ω.

3. Average field intensity outside the surface

As is known, a semiconductor can support three exciton polariton modes, of which two are transverse and one is longitudinal. We need to know which mode leads to the surface exciton polariton. In the case $\Omega > \omega_L$, $k_{1,2}$ and k_L are all real, such that the three modes may propagate in the same direction of the semiconductor. For incident frequencies Ω below ω_L, k_1 is real but k_2 and k_L are purely imaginary, such that the first transverse mode is a propagating mode while the second transverse and longitudinal modes are spatially damped. Further, the dielectric function of the longitudinal mode is identically equal to zero. Inasmuch as the surface

exciton polariton is spatially damped outside and inside the semiconductor, we conclude that the second transverse mode makes the main contribution to the surface exciton polariton. In the following the dielectric response of the semiconductor to the incident EM field is described by the dielectric function $\epsilon_2(\Omega)$ of the second transverse mode.

The system under study consists of a semi-infinite semiconductor and vacuum. The semiconductor surface is randomly rough and the ensemble average of the rough surface defines a plane surface $z = 0$. If $\mathbf{x} = (x, y)$ is the position vector of any point on the plane surface, $\zeta(\mathbf{x})$ gives the height of roughness with respect to the plane surface. Note that the three-dimensional position vector $\mathbf{r}$ is now given by $\mathbf{r} = \mathbf{x} + z\hat{z}$. Thus, the local dielectric function of the system can be written as follows:

$$\begin{aligned} &\epsilon(\mathbf{r}, \Omega) = \epsilon_0(z, \Omega) + [\epsilon_2(\Omega) - 1]\{\Theta[\zeta(\mathbf{x}) - z] - \Theta(-z)\}, \\ &\epsilon_0(z, \Omega) = \epsilon_2(\Omega)\Theta(-z) + \Theta(z), \end{aligned} \tag{11}$$

where $\Theta(z)$ is Heaviside's unit step function and $\epsilon_0(z, \Omega)$ is the local dielectric function for a plane semiconductor surface. Apparently the dielectric function $\epsilon(\mathbf{r}, \Omega)$ is a random variable near the rough surface.

$\epsilon_2(\Omega)$ given by equation (4) is negative for $\omega_T < \Omega < \omega_L$. Let a monochromatic EM beam be incident on a surface area centred at the origin $\mathbf{r} = \mathbf{0}$. The incident frequency Ω is in a frequency range larger than ω_T, so that the EM field cannot propagate in the bulk of the semiconductor. However, the incident field can excite the surface exciton polaritons near the rough surface. The macroscopic electric field $\mathbf{E}(\mathbf{r}, \Omega)$ of surface exciton polaritons satisfies the linear Maxwell equation

$$-\nabla \times \nabla \times \mathbf{E}(\mathbf{r}, \Omega) + \epsilon(\mathbf{r}, \Omega)(\Omega/c)^2\mathbf{E}(\mathbf{r}, \Omega) = 0, \tag{12}$$

which cannot be solved exactly. We need to introduce the dyadic retarded Green function $\hat{\mathbf{d}}(\mathbf{r}, \mathbf{r}', \Omega)$ of surface exciton polaritons, which obeys the equation

$$-\nabla \times \nabla \times \hat{\mathbf{d}}(\mathbf{r}, \mathbf{r}', \Omega) + \epsilon(\mathbf{r}, \Omega)(\Omega/c)^2\hat{\mathbf{d}}(\mathbf{r}, \mathbf{r}', \Omega) = \delta(\mathbf{r} - \mathbf{r}')\mathbf{I}. \tag{13}$$

With the use of this function, the electric field $\mathbf{E}(\mathbf{r}, \Omega)$ can be expressed as follows:

$$\mathbf{E}(\mathbf{r}, \Omega) = \sum_\lambda \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}[(\Omega/c)^2 - \mathbf{k}^2]E_0(\mathbf{k}, \lambda; \Omega)\mathbf{e}(\mathbf{k}, \lambda) \cdot \int \mathrm{d}\mathbf{r}' \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}'}\hat{\mathbf{d}}(\mathbf{r}', \mathbf{r}, \Omega), \tag{14}$$

$$E_0(\mathbf{k}, \lambda; \Omega) = \int \mathrm{d}\mathbf{r} \, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\mathbf{e}^*(\mathbf{k}, \lambda) \cdot \mathbf{E}_0(\mathbf{r}, \Omega), \tag{15}$$

where $\lambda = \mathrm{s}, \mathrm{p}$ characterize two polarization directions, $\mathbf{e}(\mathbf{k}, \lambda)$ is the polarization unit vector of the plane wave, and $\mathbf{E}_0(\mathbf{r}, \Omega)$ denotes the incident electric field in the infinite vacuum. The derivation of equation (14) is given in reference [18]. $\hat{\mathbf{d}}(\mathbf{r}', \mathbf{r}, \Omega)$ possesses the poles corresponding to surface exciton polaritons when $z' < 0$ and $z > 0$.

The surface polaritons exist only for the so-called transverse-magnetic wave, namely p-polarized surface polaritons. On the rough surface, however, the incident photons of s polarization can also excite the surface polaritons. The roughness coupling between the surface polaritons and the s photons is very small in the visible region and can thus be neglected [13]. In this case, we assume that the incident field is a p-polarized fundamental Gaussian beam emitted by a laser. If the distance between the laser and the origin is much greater than the distance $|\mathbf{r} \cdot \hat{k}_0|$, the incident field at the position $\mathbf{r}$ is of the form

$$\mathbf{E}_0(\mathbf{r}, \Omega) = E_0(\mathbf{0}, \Omega)\mathbf{e}(\mathbf{k}_0, p)\exp(\mathrm{i}\mathbf{k}_0 \cdot \mathbf{r} - |\mathbf{r} \times \hat{k}_0|^2/R^2), \tag{16}$$

where the wavevector $\mathbf{k}_0$ gives the incident direction and satisfies the relation $\Omega = ck_0$. R is the beam spot size at the origin and $E_0(\mathbf{0}, \Omega)$ is the incident field amplitude at the origin. Further, we suppose that equation (16) holds in the whole real space. This means that diffraction effects

of the Gaussian beam are neglected. Now we introduce the Fourier transform $\hat{\mathbf{d}}(\mathbf{n}, \mathbf{n}', \Omega|0^-0^+)$ of the Green function $\hat{\mathbf{d}}(\mathbf{r}', \mathbf{r}, \Omega)$ on the surface with respect to $\mathbf{x}'$ and $\mathbf{x}$. Consequently, the electric field $\mathbf{E}(\mathbf{r}, \Omega)$ outside the surface excited by the Gaussian beam can be expressed as follows:

$$\mathbf{E}(\mathbf{r}, \Omega) = \int \frac{\mathrm{d}\mathbf{n}}{(2\pi)^2} \int \frac{\mathrm{d}\mathbf{n}'}{(2\pi)^2} A(\mathbf{n}, \Omega) \mathrm{e}^{\mathrm{i}\mathbf{n}'\cdot\mathbf{x} - k_2(\mathbf{n}')z} \mathbf{e}(\mathbf{n}, p) \cdot \hat{\mathbf{d}}(\mathbf{n}, \mathbf{n}', \Omega|0^-0^+), \tag{17}$$

$$A(\mathbf{n}, \Omega) = -E_0(\mathbf{0}, \Omega)\pi R^2 \mathrm{e}^{-R^2(n - k_0 \sin\theta)^2/4\cos^2\theta} \frac{k_0(n - k_0 \sin\theta)^2}{|\mathbf{n} - \mathbf{k}_0|[\mathrm{i}(n \sin\theta - k_0) + k_1(\mathbf{n}) \cos\theta]}, \tag{18}$$

$$k_1(\mathbf{n}) = [n^2 - \epsilon_2(\Omega)\Omega^2/c^2]^{1/2}, \qquad k_2(\mathbf{n}) = (n^2 - \Omega^2/c^2)^{1/2}. \tag{19}$$

$$\mathbf{e}(\mathbf{n}, p) = \frac{n \cos\theta}{|\mathbf{n} - \mathbf{k}_0|} \hat{z} - \frac{n \sin\theta - k_0}{|\mathbf{n} - \mathbf{k}_0|} \hat{n},$$

where θ is the incident angle. $A(\mathbf{n}, \Omega)$ and $\mathbf{e}(\mathbf{n}, p)$ can be regarded as the wave amplitude and polarization vector of surface exciton polaritons. The derivation of equation (17) is given in [7].

In optical experiments, what we can detect directly is the average EM field intensity of surface exciton polaritons outside the surface. Theoretically, the average field intensity is determined by the field correlation function, which is defined as

$$\begin{aligned}\langle E_j(\mathbf{r}, \Omega + \omega) E_l^*(\mathbf{r}', \Omega)\rangle = {} & \int \frac{\mathrm{d}\mathbf{q}}{(2\pi)^2} \int \frac{\mathrm{d}\mathbf{n}}{(2\pi)^2} \int \frac{\mathrm{d}\mathbf{n}'}{(2\pi)^2} \int \frac{\mathrm{d}\mathbf{n}''}{(2\pi)^2} A(\mathbf{n}^+, \Omega + \omega) A^*(\mathbf{n}^-, \Omega) \\ & \times \mathrm{e}^{\mathrm{i}\mathbf{n}'^+\cdot\mathbf{x} - k_2(\mathbf{n}'^+)z - \mathrm{i}\mathbf{n}''^-\cdot\mathbf{x}' - k_2^*(\mathbf{n}''^-)z'} \sum_{i,k} e_i(\mathbf{n}^+, p) e_k^*(\mathbf{n}^-, p) \\ & \times \langle \hat{d}_{ij}(\mathbf{n}^+, \mathbf{n}'^+; \Omega + \omega|0^-0^+) \hat{d}_{kl}^*(\mathbf{n}^-, \mathbf{n}''^-; \Omega|0^-0^+)\rangle, \end{aligned} \tag{20}$$

where $\mathbf{n}^\pm = \mathbf{n} \pm \mathbf{q}/2$ and for convenience $\mathbf{q}$ is supposed to vary only near the origin $\mathbf{q} = \mathbf{0}$. The brackets $\langle \cdots \rangle$ indicate an ensemble average over all possible configurations of the rough surface. Equation (20) shows that the field correlation function is connected with the average two-particle Green function in momentum space. In the limit $\omega \to 0$ and in the case $\mathbf{r} = \mathbf{r}'$, $j = l$, the field correlation function gives the average field intensity $\langle |\mathbf{E}(\mathbf{r}, \Omega)|^2 \rangle$ outside the surface.

4. Localization theory of surface exciton polaritons

Our goal is to prove the localization of surface exciton polaritons in the sense that the diffusion coefficient of the EM energy vanishes. Therefore, the study of localization involves the evaluation of the average one- and two-particle Green functions in momentum space. We will proceed within the framework of multiple-scattering theory. At first, we notice that the average one-particle Green function in momentum space has the diagonal form

$$\langle \hat{\mathbf{d}}(\mathbf{n}, \mathbf{n}', \Omega|0^-0^+)\rangle = (2\pi)^2 \delta(\mathbf{n} - \mathbf{n}') \mathbf{d}(\mathbf{n}, \Omega|0^-0^+). \tag{21}$$

Next, we suppose that the surface configurations satisfy a Gaussian distribution. This means that the configuration function $\zeta(\mathbf{x})$ has the ensemble average value $\langle \zeta(\mathbf{x})\zeta(\mathbf{x}')\rangle = \delta^2 \mathrm{e}^{-(\mathbf{x}-\mathbf{x}')^2/a^2}$, where δ is the root-mean-square roughness amplitude and a is the transverse correlation length. In the following we concentrate on the small roughness case. The assumption of small roughness means that the root-mean-square δ shall be much smaller than the wavelength λ of the incident light: $\delta \ll \lambda$.

Under the assumption of small roughness, within the framework of the average T-matrix approximation, the diagonal average one-particle Green function meets the Dyson equation [7]

$$\mathbf{d}(\mathbf{n}, \Omega|0^-0^+) = \mathbf{d}_0(\mathbf{n}, \Omega|0^-0^+) + \mathbf{d}_0(\mathbf{n}, \Omega|0^-0^+) \cdot \boldsymbol{\Sigma}(\mathbf{n}, \Omega|0^-0^+) \cdot \mathbf{d}(\mathbf{n}, \Omega|0^-0^+). \tag{22}$$

$\mathbf{d}_0(\mathbf{n}, \Omega|0^-0^+)$ is the unperturbed Green function in momentum space and $\mathbf{\Sigma}(\mathbf{n}, \Omega|0^-0^+)$ is the self-energy function in momentum space given by

$$\mathbf{\Sigma}(\mathbf{n}, \Omega|0^-0^+) = w^2(\Omega)\delta^2 \int \frac{\mathrm{d}\mathbf{n}'}{(2\pi)^2} g(\mathbf{n}' - \mathbf{n})\mathbf{d}_0(\mathbf{n}', \Omega|0^-0^+), \tag{23}$$

where $w(\Omega) = [1 - \epsilon_2(\Omega)](\Omega/c)^2$ and $g(\mathbf{n}) = \pi a^2 \exp(-a^2n^2/4)$. Once $\mathbf{d}_0(\mathbf{n}, \Omega|0^-0^+)$ is known, $\mathbf{d}(\mathbf{n}, \Omega|0^-0^+)$ can be evaluated from equations (22) and (23). Reference [19] outlines the derivation of the unperturbed Green function $\mathbf{d}_0$. The unperturbed Green function in momentum space can be written as follows:

$$\mathbf{d}_0(\mathbf{n}, \Omega|0^-0^+) = d_0(\mathbf{n}, \Omega)\mathbf{e}^-(\mathbf{n}, \Omega)\mathbf{e}^+(\mathbf{n}, \Omega), \tag{24}$$

$$d_0(\mathbf{n}, \Omega) = -\frac{c^2n^2}{\Omega^2} \frac{1}{k_1(\mathbf{n}) + k_2(\mathbf{n})\epsilon_2(\Omega)}, \tag{25}$$

$$\mathbf{e}^-(\mathbf{n}, \Omega) = \hat{z} + \mathrm{i}\frac{k_1(\mathbf{n})}{n}\hat{n}, \qquad \mathbf{e}^+(\mathbf{n}, \Omega) = \hat{z} + \mathrm{i}\frac{k_2(\mathbf{n})}{n}\hat{n}. \tag{26}$$

Here $k_1(\mathbf{n})$ and $k_2(\mathbf{n})$ are given by equation (19). If $\omega_\mathrm{T} < \Omega < \omega_\mathrm{L}$ and $n > \Omega/c$, $k_1(\mathbf{n})$ and $k_2(\mathbf{n})$ are real and positive, and so $d_0(\mathbf{n}, \Omega)$ represents the unperturbed Green function of surface exciton polaritons. Inasmuch as the dielectric function $\epsilon_2(\Omega)$ given by equation (4) is negative, the dispersion relation of surface exciton polaritons can be determined by the equation of poles of the unperturbed Green function $d_0(\mathbf{n}, \Omega)$. Using equation (19) for $k_1(\mathbf{n})$ and $k_2(\mathbf{n})$, from equation (25) one can rewrite the unperturbed Green function of surface exciton polaritons into the standard form:

$$d_0(\mathbf{n}, \Omega) = \frac{\alpha(n, \Omega)}{\Omega - \Omega(n) + \mathrm{i}\Gamma_\mathrm{s}}, \tag{27}$$

$$\alpha(n, \Omega) = \frac{c^4n^2[k_1(\mathbf{n}) - k_2(\mathbf{n})\epsilon_2(\Omega)]}{\Omega^2\epsilon_2(\Omega)[1 - \epsilon_2(\Omega)][\Omega + \Omega(n)]}, \tag{28}$$

where $\Omega(n)$ is the real part of the complex frequency of surface exciton polaritons determined by equation (9).

Likewise, the average one-particle Green function in momentum space can be written as

$$\mathbf{d}(\mathbf{n}, \Omega|0^-0^+) = d(\mathbf{n}, \Omega)\mathbf{e}^-(\mathbf{n}, \Omega)\mathbf{e}^+(\mathbf{n}, \Omega). \tag{29}$$

Putting equations (24) and (29) into equation (22), we obtain the Dyson equation for $d(\mathbf{n}, \Omega)$:

$$d(\mathbf{n}, \Omega) = d_0(\mathbf{n}, \Omega) + d_0(\mathbf{n}, \Omega)\Sigma_t(n, \Omega)d(\mathbf{n}, \Omega), \tag{30}$$

$$\Sigma_t(n, \Omega) = \mathbf{e}^+(\mathbf{n}, \Omega) \cdot \mathbf{\Sigma}(\mathbf{n}, \Omega|0^-0^+) \cdot \mathbf{e}^-(\mathbf{n}, \Omega). \tag{31}$$

In the small roughness case, the energy change of surface exciton polaritons due to disorder can be omitted, so the dispersion relation $\Omega = \Omega(n)$ holds. We keep only the imaginary part γ of the self-energy. The average one-particle Green function of surface exciton polaritons is calculated from equations (27) and (30) as

$$d(\mathbf{n}, \Omega) = \frac{\alpha(n, \Omega)}{\Omega - \Omega(n) + \mathrm{i}(\gamma + \Gamma_\mathrm{s})}, \tag{32}$$

where $\gamma = -\alpha(n_\mathrm{s}, \Omega)\ \mathrm{Im}\ \Sigma_t(n_\mathrm{s}, \Omega)$ and $n = n_\mathrm{s}(\Omega)$ is the solution of the dispersion relation (9) of surface exciton polaritons. The physical meaning of γ can be seen if we let $\gamma = \gamma_\mathrm{el} + \gamma_\mathrm{rad}$. γ_el is the elastic scattering rate from the state $\mathbf{n}_\mathrm{s}(\Omega)$ into other states $\mathbf{n}'_\mathrm{s}(\Omega)$, and γ_rad represents the radiative rate from the surface polariton state into p-photon modes of $n < \Omega/c$.

γ_el and γ_rad can be found by the technique recounted in [7]. After lengthy calculation, we have obtained the concrete expression of γ_el:

$$\gamma_\mathrm{el} = (\Omega/c)^4\{\pi[1 - \epsilon_2(\Omega)]\delta a\alpha(n_\mathrm{s}, \Omega)\}^2 N(\Omega) f(\Omega) \exp(-a^2n_\mathrm{s}^2/2), \tag{33}$$

$$f(\Omega) = [1 + k_1^2(n_\mathrm{s})k_2^2(n_\mathrm{s})/2n_\mathrm{s}^4]I_0(a^2n_\mathrm{s}^2/2) - 2k_1(n_\mathrm{s})k_2(n_\mathrm{s})I_1(a^2n_\mathrm{s}^2/2)/n_\mathrm{s}^2 + k_1^2(n_\mathrm{s})k_2^2(n_\mathrm{s})I_2(a^2n_\mathrm{s}^2/2)/2n_\mathrm{s}^4,$$

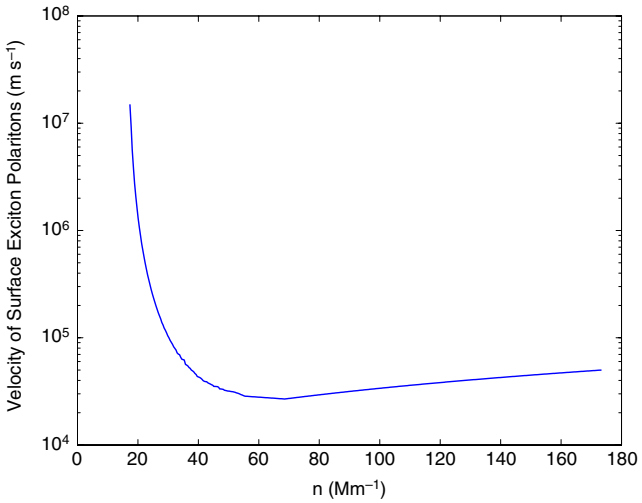

Figure 3. Variation of the velocity of surface exciton polaritons with wavevector n.

where $I_n(z)$ is the modified Bessel function of the first kind of order n. $N(\Omega) = n_s(\Omega)/2\pi v(n_s)$ is the surface polariton density of states near frequency Ω and $v(n) = \mathrm{d}\Omega(n)/\mathrm{d}n$ is the velocity of surface exciton polaritons. With the approximation $v(n) = \Delta\Omega(n)/\Delta n$, the numerical values of the velocity can be easily derived from figure 1. Figure 3 shows the variation of the velocity v with wavevector n. First v decreases rapidly with increasing n and then it increases gently with n. Likewise, γ_{rad} has been obtained as follows:

$$\gamma_{\mathrm{rad}} = -\tfrac{1}{2}\{(\Omega/c)[1-\epsilon_2(\Omega)]\delta a\}^2\alpha(n_s,\Omega)u(\Omega)\exp(-a^2n_s^2/4), \tag{34}$$

$$u(\Omega) = \int_0^{\Omega/c} \mathrm{d}n' \exp(-a^2n'^2/4)\frac{n'^3k_3(n')h(n',\Omega)}{k_1^2(n')+k_3^2(n')\epsilon_2^2(\Omega)},$$

$$\begin{aligned} h(n,\Omega) = {} & [k_1(n_s)k_2(n_s)k_1^2(n)/2n_s^2n^2 - \epsilon_2(\Omega)]I_0(a^2n_sn/2) \\ & + [k_2(n_s)\epsilon_2(\Omega) - k_1(n_s)]k_1(n)I_1(a^2n_sn/2)/n_sn \\ & + k_1(n_s)k_2(n_s)k_1^2(n)I_2(a^2n_sn/2)/2n_s^2n^2, \end{aligned}$$

where $k_3(\mathbf{n}) = (\Omega^2/c^2 - n^2)^{1/2}$. The numerical calculation shows that γ_{rad} is much smaller than γ_{el}. Therefore, in the following discussion, we consider only $d(\mathbf{n},\Omega)$ of $n > \Omega/c$.

Similar to the average one-particle Green function, the average two-particle Green function in momentum space has the general form

$$\begin{aligned} \langle\hat{d}_{ij}(\mathbf{n}^+,\mathbf{n}'^+;\Omega+\omega|0^-0^+)\hat{d}^*_{kl}(\mathbf{n}^-,\mathbf{n}''^-;\Omega|0^-0^+)\rangle = {} & (2\pi)^2\delta(\mathbf{n}'-\mathbf{n}'')e_i^-(\mathbf{n}^+,\Omega+\omega)e_j^+ \\ & \times(\mathbf{n}'^+,\Omega+\omega)e_k^{-*}(\mathbf{n}^-,\Omega)e_l^{+*}(\mathbf{n}'^-,\Omega)T(\mathbf{n},\mathbf{n}';\Omega,\mathbf{q},\omega), \end{aligned} \tag{35}$$

where $\mathbf{n}^\pm = \mathbf{n}\pm\mathbf{q}/2$ and T satisfies a scalar Bethe–Salpeter equation. We introduce the density relaxation function of surface exciton polaritons by

$$T(\Omega,\mathbf{q},\omega) = \int\frac{\mathrm{d}\mathbf{n}}{(2\pi)^2}\int\frac{\mathrm{d}\mathbf{n}'}{(2\pi)^2}T(\mathbf{n},\mathbf{n}';\Omega,\mathbf{q},\omega). \tag{36}$$

With the mathematical technique developed by Vollhardt and Wölfle [20], it follows that the density relaxation function meets the diffusion equation ($q\to 0, \omega\to 0$):

$$T(\Omega,\mathbf{q},\omega) = \frac{2\pi\mathrm{i}\alpha^2(n_s,\Omega)N(\Omega)}{\omega+\mathrm{i}D(\mathbf{q},\omega)q^2}. \tag{37}$$

In the preceding discussion, we neglect inelastic scattering effects due to radiation of surface exciton polaritons, dissipation of excitons, and spatial dispersion of excitons. $\gamma_{\rm rad}$ represents the radiative effect. Excitonic dissipation originates from exciton radiation and phonon scattering. In the empirical theory, one describes the excitonic dissipative effect by replacing Ω^2 with $\Omega(\Omega + {\rm i}\Gamma)$ in the dielectric function given by equation (1), where Γ is called the exciton damping constant. $\Gamma_{\rm s}$ signifies the spatial dispersion effect. Therefore, the inelastic scattering rate of surface exciton polaritons is $\gamma_{\rm inel} = \gamma_{\rm rad} + \Gamma + \Gamma_{\rm s}$. In equation (37) we can include the inelastic scattering effects via the replacement $\omega \to \omega + {\rm i}\gamma_{\rm inel}$. $D(\mathbf{q}, \omega)$ is the renormalized diffusion coefficient and is given by

$$D(\mathbf{q}, \omega) = D_0 \left[1 - \frac{1}{\pi n_{\rm s}(\Omega) l_{\rm el}} \int_0^{n_{\rm c}} {\rm d}n \frac{2n}{n^2 - {\rm i}(\omega + {\rm i}\gamma_{\rm inel})/D(\mathbf{q}, \omega)} \right], \tag{38}$$

where $D_0 = v^2(n_{\rm s})/4\gamma_{\rm el}$ is the bare diffusion coefficient. We have introduced an upper cutoff $n_{\rm c} = \sqrt{(l_{\rm el} l_{\rm inel})^{-1} - \xi^{-2}}$ into the integration, where

$$l_{\rm el} = v(n_{\rm s})/2\gamma_{\rm el} \qquad \text{and} \qquad l_{\rm inel} = v(n_{\rm s})/2\gamma_{\rm inel} \tag{39}$$

are the elastic and inelastic mean free path of surface exciton polaritons, respectively, and ξ is a characteristic length.

Anderson pointed out that the envelope of the wavefunction of a localized electron decays exponentially from some point in space, $|\psi(\mathbf{r})| \sim \exp(-|\mathbf{r} - \mathbf{r}_0|/\xi)$, where ξ is called the localization length of electron. The Anderson localization means that in the limit $\omega \to 0$, $D(\mathbf{q}, \omega) \to 0$. Thereby we define the characteristic length $\xi = \lim_{\omega \to 0} ({\rm i}D/\omega)^{1/2}$. We shall show that the intensity of localized surface exciton polaritons behaves as $\langle |\mathbf{E}(\mathbf{x}, \Omega)|^2 \rangle \sim \exp(-|\mathbf{x}|/\xi)$, so that ξ is the localization length of surface exciton polaritons. As a result of equation (38), the localization length is given by

$$\xi^2 = \frac{l_{\rm el} l_{\rm inel} \exp[\pi n_{\rm s}(\Omega) l_{\rm el}]}{2 - \exp[\pi n_{\rm s}(\Omega) l_{\rm el}]}. \tag{40}$$

ξ is real and positive only if the denominator on the right-handed side of equation (40) is positive. Equation (40) always supports the solution of a positive real ξ in the frequency range of interest. $\xi \propto \exp[\frac{1}{2}\pi n_{\rm s}(\Omega) l_{\rm el}]$ is found from the last equation. We require that the localization length ξ is larger than the elastic mean free path $l_{\rm el}$ and the elastic mean free path $l_{\rm el}$ cannot be much shorter than the transverse correlation length a. Inasmuch as the inelastic scattering effects always tend to destroy the elastic scattering effects, the localization is meaningful only if $l_{\rm el} \ll l_{\rm inel}$. Consequently, the criteria for the localization of surface exciton polaritons are that $\xi > l_{\rm el}$, $l_{\rm el} \ll l_{\rm inel}$, and $l_{\rm el}/a > 0.1$. On the other hand, elastic scattering from the rough surface is ineffective if $l_{\rm el}/a \leqslant 0.1$, such that the surface polaritons are in extended states. In this case, in the limit $\omega \to 0$ the renormalized diffusion coefficient is given by

$$D(\mathbf{q}, 0) = D_0 \left[1 - \frac{1}{\pi n_{\rm s}(\Omega) l_{\rm el}} \int_0^{n_{\rm c}} {\rm d}n \frac{2n}{n^2 + (l_{\rm el} l_{\rm inel})^{-1}} \right], \tag{41}$$

where we have introduced an upper cutoff $n_{\rm c} = 1/l_{\rm inel}$ into the integration. After the integration is carried out, the renormalized diffusion coefficient is $D(\mathbf{q}, 0) = D_0(1 - \eta/l_{\rm el})$ with the delocalization length

$$\eta = \frac{\ln(1 + l_{\rm el}/l_{\rm inel})}{\pi n_{\rm s}(\Omega)}. \tag{42}$$

The delocalization length η must be smaller than the elastic mean free path $l_{\rm el}$.

From equation (20) we show that for the Gaussian incident beam, the field correlation function outside the surface is completely determined by the density relaxation function defined in equation (36), i.e.,

$$\langle \mathbf{E}(\mathbf{r}, \Omega + \omega) \cdot \mathbf{E}^*(\mathbf{r}, \Omega) \rangle \propto \mathrm{e}^{-2k_2(n_s)z} \int \frac{\mathrm{d}\mathbf{q}}{(2\pi)^2} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{x}} T(\Omega, \mathbf{q}, \omega). \tag{43}$$

This means that the Gaussian incident beam can produce the localization of surface polaritons. We have found $T(\Omega, \mathbf{q}, \omega)$ as given by equation (37) with the replacement $\omega \to \omega + \mathrm{i}\gamma_{\mathrm{inel}}$. Equations (37) and (43) are obtained for small q and ω. If equation (37) is put into equation (43), the integral variable $\mathbf{q}$ can resume varying on the whole wavevector plane because the main contribution to the $\mathbf{q}$ integration comes from the small q region. When the $\mathbf{q}$ integration is carried out in the limit $\omega \to 0$, equation (43) can be written as $\langle |\mathbf{E}(\mathbf{r}, \Omega)|^2 \rangle = |E_0(\mathbf{0}, \Omega)|^2 \rho(\mathbf{r}, \Omega)$. Here $|E_0(\mathbf{0}, \Omega)|^2$ is the incident field intensity at the origin. $\rho(\mathbf{r}, \Omega)$ denotes the enhancement of the field intensity outside the surface and is given by

$$\rho(\mathbf{r}, \Omega) = \rho_0(\Omega) \mathrm{e}^{-2k_2(n_s)z} K_0(|\mathbf{x}|/l) \qquad \text{for } |\mathbf{x}| > l_{\mathrm{el}}, \tag{44}$$

where $K_0(x)$ is the modified Bessel function of the second kind of order zero and

$$\rho_0(\Omega) = \alpha^2(n_s, \Omega) N(\Omega) [1 + k_2^2(n_s)/n_s^2(\Omega)] \frac{|A(n_s, \Omega)|^2}{|E_0(0, \Omega)|^2} \times \frac{n_s^4(\Omega) \cos^2\theta + k_1^2(n_s)[n_s(\Omega)\sin\theta - k_0]^2}{D_0 n_s^2(\Omega) |\mathbf{n}_s(\Omega) - \mathbf{k}_0|^2}. \tag{45}$$

l represents the decaying length of the field in the xy plane and is given by

$$l = \begin{cases} (l_{\mathrm{el}} l_{\mathrm{inel}})^{1/2} & \text{in extended states,} \\ \xi \left(\dfrac{l_{\mathrm{el}} l_{\mathrm{inel}}}{\xi^2 + l_{\mathrm{el}} l_{\mathrm{inel}}} \right)^{1/2} & \text{in localized states.} \end{cases} \tag{46}$$

The decaying length in extended states is always larger than that in localized states.

5. Numerical results

To make the numerical calculation, we select a single crystal of ZnO as the semi-infinite semiconductor. One of the reasons for this selection is that the exciton-free surface layer of ZnO is less than about 30 Å, probably the smallest one of the II–VI semiconducting compounds. Another reason is that ZnO semiconductors were used for the first observation of surface exciton polaritons. ZnO has the wurtzite structure. Therefore, two exciton transition series are polarized perpendicular to the hexagonal c-axis (A and B excitons) and one polarized parallel to the c-axis (C excitons). The differently polarized transitions with main quantum number $n = 1$ are separated by about 40 meV. We suppose that the influence of the $A_{n=1}$ and $B_{n=1}$ excitons in the energy range of the differently polarized $C_{n=1}$ exciton is not too important and hence can be omitted. Thus, we assume an isotropic medium. In section 2, we give most of the known data of the $C_{n=1}$ exciton of ZnO. For the following calculations one still needs the exciton damping constant, which is $\Gamma = 0.5$ meV [17]. Since the surface roughness of the ZnO semiconductor can be controlled at will, the transverse correlation length a is chosen equal to 47.68 nm. In a frequency range near ω_{L}, the wavelength λ of the incident light has an order of magnitude of 362 nm. For the root-mean-square roughness amplitude we use the value $\delta = 47$ nm, so that the small roughness condition $\delta \ll \lambda$ is met. The beam spot size of the incident light at the origin is required to be less than the light wavelength, so that we choose a very small value $R = 0.197\ \mu$m. The reason for the requirement is that if the beam spot size R

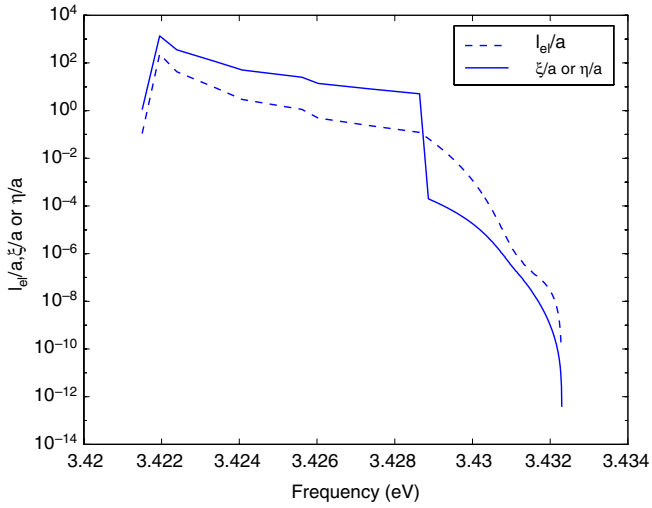

Figure 4. Frequency dependence of the elastic mean free path $l_{\rm el}$, localization length ξ, and delocalization length η in units of the transverse correlation length a.

is larger than the light wavelength λ, interference effects are inessential on the rough surface, whereas the localization is just due to strong interference effects.

We first examine the characteristics of the localization of surface exciton polaritons. The numerical analysis will use equations (39), (40), and (42). The parameters $l_{\rm el}$, ξ, η, and $l_{\rm el}/l_{\rm inel}$ are calculated in a frequency range $\omega_{\rm T} \leqslant \Omega \leqslant \omega_{\rm L}$ for $\delta = 47$ nm, and the numerical results are depicted, respectively, in figures 4 and 5. As shown, for a fixed $\delta = 47$ nm, there is a mobility edge $\Omega^* = 3.4288$ eV, which is determined by the condition $l_{\rm el}/a = 0.1$. In the frequency range between $\omega_{\rm T}$ and Ω^*, $l_{\rm el}/a > 0.1$ and $\xi > l_{\rm el}$, while in the frequency range between Ω^* and $\omega_{\rm L}$, $l_{\rm el}/a < 0.1$ and $\eta < l_{\rm el}$. Further, $l_{\rm el} \ll l_{\rm inel}$ in the whole frequency range. Consequently, the localization appears in a limited frequency range above $\omega_{\rm T}$. The localization length ξ describes the degree of localization; the smaller ξ is, the larger the degree of localization is. In the limit $\Omega \to \omega_{\rm T}$, the exciton–polariton is called a resonantly excited exciton. Almost resonantly excited excitons are real quasiparticles that can be trapped and localized by surface roughness. Resonantly excited excitons in a single GaAs quantum well reveal an enhanced radiative recombination in comparison with the three-dimensional excitons [21]. It has been found that such a radiative decay is much slowed by localization [22]. We expect that resonantly excited excitons on a rough surface will show a much slower radiative decay, due to localization. When Ω approaches $\omega_{\rm L}$, the exciton–polariton is still exciton-like. We notice that $l_{\rm el} \propto [\epsilon_2(\Omega)]^2$. In the limit $\Omega \to \omega_{\rm L}$, since the dielectric function $\epsilon_2(\Omega)$ approaches zero, the rapid decrease of $l_{\rm el}/a$ inhibits the localization of surface exciton polaritons.

Next we must analyse the enhancement of the field intensity outside the surface. The limiting form of $K_0(x)$ at $x \gg 1$ is $K_0(x) \to (\pi/2x)^{1/2}{\rm e}^{-x}$. This shows that the field of surface exciton polaritons is confined within a radius from the z-axis. The confined behaviour of the field on the surface is due to multiple scattering effects. The limiting form of $K_0(x)$ at $x \ll 1$ is $K_0(x) \to -\ln(x/2) - 0.5772$. In mathematics the field intensity seems to be infinite at the origin, but in physics the field intensity is finite at the origin. Inasmuch as equation (43) is derived under the diffusion assumption, it is true only at the propagation distance $|\mathbf{x}| > l_{\rm el}$. For $|\mathbf{x}| < l_{\rm el}$, the propagation is basically wavelike and hence equation (43) is ineffective. The calculation reveals that $l_{\rm el} < 11.23\ \mu$m for $\omega_{\rm T} \leqslant \Omega \leqslant \omega_{\rm L}$. In the frequency range between

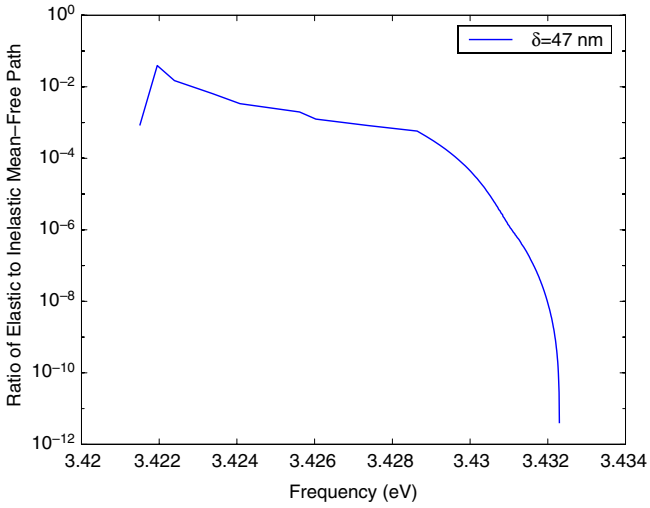

Figure 5. Frequency dependence of the ratio $l_{\rm el}/l_{\rm inel}$ of the elastic to the inelastic mean free path, for $\delta = 47$ nm.

$\omega_{\rm T}$ and $\omega_{\rm L}$, the field intensity in the small area of $|\mathbf{x}| \leqslant l_{\rm el}$ can be approximated as a constant. Since the field intensity is continuous across $|\mathbf{x}| = l_{\rm el}$, we write

$$\rho(\mathbf{r}, \Omega) = \rho_0(\Omega) \mathrm{e}^{-2k_2(n_{\rm s})z} K_0(l_{\rm el}/l) \qquad \text{for } |\mathbf{x}| \leqslant l_{\rm el}. \tag{47}$$

The peak of the variation of the enhancement $\rho(\mathbf{r}, \Omega)$ with $\mathbf{r}$ appears in the wave region $|\mathbf{x}| \leqslant l_{\rm el}$ on the surface $z = 0^+$. Therefore the enhancement peak is given by

$$\rho_{\rm p} = \rho_0(\Omega) K_0(l_{\rm el}/l), \tag{48}$$

where $l_{\rm el}$ represents the peak radius of surface exciton polaritons and $\rho_0(\Omega)$ is given by equation (45). The enhancement peak $\rho_{\rm p}$ depends on the frequency Ω, roughness amplitude δ, and incident angle θ.

The following numerical analysis will use equation (48). Figure 6 shows the variation of $\rho_{\rm p}$ with Ω at $\delta = 47$ nm and $\theta = 8.1°$. For a fixed δ, $\rho_{\rm p}$ decreases first with increasing Ω, comes to a minimum around 3.422 eV, then increases with increasing Ω, reaches a maximum around 3.4306 eV, and finally decreases steeply. In the localized region where $\omega_{\rm T} \leqslant \Omega < \Omega^*$, $\rho_{\rm p}$ is always larger than unity, i.e., the field intensity of surface exciton polaritons is enhanced relative to the incident intensity. The enhancement mechanism here is as follows. As the surface exciton polaritons in localized states cannot propagate on the surface, the energy of the incident light must accumulate on the surface, which produces the following two results. (1) The peak radius of surface exciton polaritons can be larger than the beam spot size of the incident light and (2) the field intensity of surface exciton polaritons is larger than the incident intensity. In the extended region where $\Omega^* \leqslant \Omega \leqslant \omega_{\rm L}$, $\rho_{\rm p}$ can be much larger than unity, i.e., the field intensity of surface exciton polaritons can be greatly enhanced relative to the incident intensity. The maximum enhancement here is of the order of 10^{12}. In contrast the maximum enhancement of surface phonon (plasmon) polaritons is just of the order of 10^2. The enhancement mechanism here is that the peak radius $l_{\rm el}$ of surface exciton polaritons is far smaller than the beam spot size R of the incident light. The energy conservation requires that the field intensity of surface exciton polaritons be extremely larger than the incident intensity. It is interesting to notice that the field intensity of surface exciton polaritons is practically equal to zero when $l_{\rm el}/R = 1.39 \times 10^{-7}$.

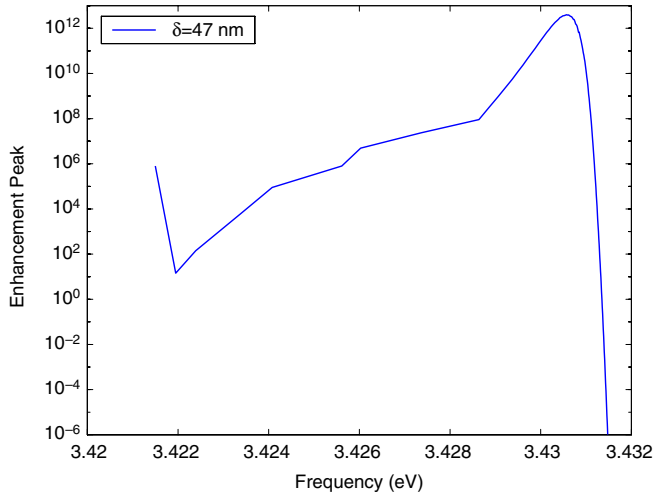

Figure 6. Frequency dependence of the enhancement peak ρ_p in the field intensity at $\delta = 47$ nm and $\theta = 8.1°$.

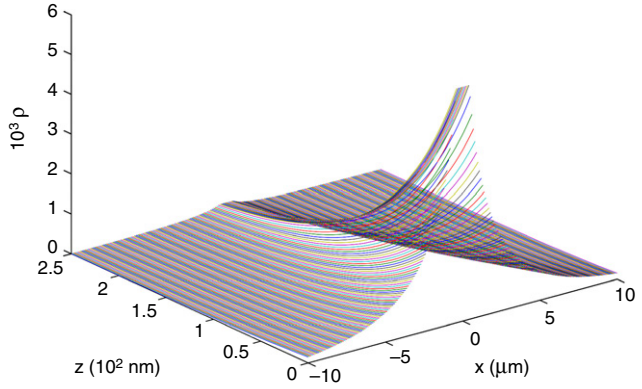

Figure 7. Distribution of the enhancement $\rho(\mathbf{r}, \Omega)$ in the field intensity in the x–z plane, with $\Omega = 3.4234$ eV, $\delta = 47$ nm, and $\theta = 8.1°$.

The following numerical analysis will use equations (44) and (47). In figure 7, we show the distribution of the enhancement $\rho(\mathbf{r}, \Omega)$ in the x–z plane for $\Omega = 3.4234$ eV, $\delta = 47$ nm, and $\theta = 8.1°$. These parameters correspond to a localized state, in which $l = 3.9228$ μm, $l_{el} = 0.4439$ μm, $[2k_2(n_s)]^{-1} = 77.3947$ nm, and $\rho_0(\Omega) = 2.5518 \times 10^3$. Figure 7 reveals that the enhancement peak ρ_p is about twice as large as $\rho_0(\Omega)$, because of $l \gg l_{el}$. Further, the decay of the field intensity on the surface is much smaller than that away from the surface, because of $l \gg [2k_2(n_s)]^{-1}$. The field intensity is, therefore, confined in the surface area of a small radius l_{el} centred at the incident point, with a large enhancement. This is similar to the field intensity of surface phonon (plasmon) polaritons in localized states.

6. Discussion

Now it is time for us to address the relations and differences between results produced by the incident Gaussian beam and plane wave. As we have seen, the electric field of the

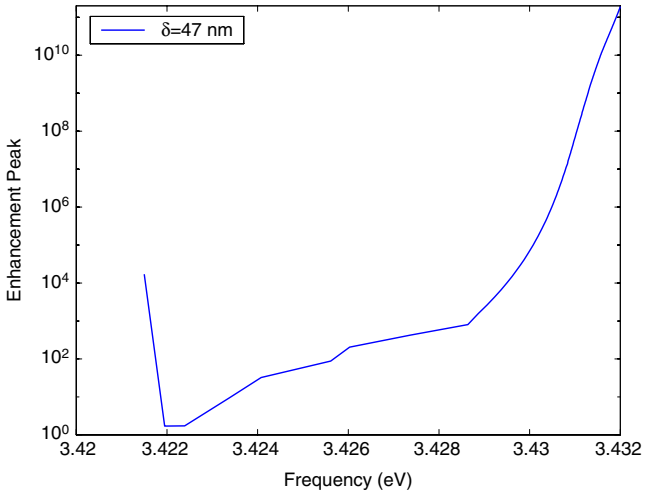

Figure 8. Frequency dependence of the enhancement peak ρ_{p} in the field intensity of plane waves. All the parameters and illustrations are the same as in figure 6.

incident Gaussian beam and the excited electric field outside the semiconductor surface are given by equations (16) and (17), respectively. Provided that the light source emitting a plane wave possesses a circular aperture stop of radius R and the wave's diffraction effects can be neglected, the electric field of the incident plane wave reads

$$\mathbf{E}_0(\mathbf{r}, \Omega) = E_0(0, \Omega)\mathbf{e}(\mathbf{k}_0, p)S(\mathbf{r}) \exp(\mathrm{i}\mathbf{k}_0 \cdot \mathbf{r}), \tag{49}$$

where $S(\mathbf{r}) = 1$ if $|\mathbf{r} \times \hat{k}_0| \leqslant R$ or zero otherwise. The electric field excited by the incident plane wave is still given by equation (17) but the function $A(\mathbf{n}, \Omega)$ has the following form:

$$A(\mathbf{n}, \Omega) = -E_0(0, \Omega)\pi R^2 \frac{k_0(n - k_0 \sin\theta)^2}{|\mathbf{n} - \mathbf{k}_0|[\mathrm{i}(n \sin\theta - k_0) + k_1(\mathbf{n}) \cos\theta]}. \tag{50}$$

In comparison with equation (18), equation (50) lacks a decaying exponential factor. If we continue to discuss the scattering properties of plane waves, then all the physical quantities have the same expressions as those of Gaussian beams. Therefore, the theoretical framework of the scattering of Gaussian beams admits the scattering of plane waves. The localization behaviour of plane waves is identical to that of Gaussian beams. For example, figures 4 and 5 completely apply to plane waves in quality and quantity. However, the dependence of the field intensity of plane waves on the radius R, the incident angle θ, and the frequency Ω is different from that of Gaussian beams. Both are identical only if $R^2(n_{\mathrm{s}} - k_0 \sin\theta)^2 \ll 2\cos^2\theta$. Under the same conditions as figure 6 and using equation (48), figure 8 shows the frequency dependence of the enhancement peak ρ_{p} in the field intensity of plane waves. Quantitative changes in the field intensity of plane waves are tremendous compared with that of Gaussian beams. The enhancement peak ρ_{p} first decreases and then increases on increasing of the frequency Ω. The substitution of plane waves for Gaussian beams can decrease the intensity enhancement by the order of 10.

In three-dimensional disordered systems without confinement, diffraction effects of light will conceal the localization effects, so that the localization effects are hard to observe. However, surface exciton polaritons are confined to a two-dimensional system and the localization condition can be easily satisfied in realistic experimental situations. The localization effects are embodied in the large enhancement and fast decay of the field intensity

on the surface and they will be observed in surface optical experiments. The real part of the complex frequency of surface exciton polaritons has an order of magnitude of 3 eV, while its imaginary part has an order of magnitude of -1 meV. The numerical calculation shows that the imaginary part of the complex frequency of surface exciton polaritons does not prevent the observation of localization of surface exciton polaritons. The beam spot size of incident laser light has a typical value $R = 0.197$ μm, which is smaller than the light wavelength. Current laser technology is certain to produce such a beam of laser light.

The present paper develops a numerical model to investigate the localization of surface exciton polaritons in the presence of random roughness and spatial dispersion. It is found that the localization occurs in a limited frequency range above the resonant frequency ω_{T} of transverse excitons. Given Ω^* is the mobility edge, as a universal law, the localization dominates the spectrum range $\omega_{\mathrm{T}} \leqslant \Omega \leqslant \Omega^*$. In localized states the field intensity of surface exciton polaritons is enhanced greatly and is much higher than that of surface phonon (plasmon) polaritons. The localization of surface exciton polaritons is due to the destructive interference between waves scattered from the rough surface. In conclusion, we establish the localization theory of Gaussian laser beams and plane light waves on a rough semiconductor surface.

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