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Electromagnetic enhancement effect in scanning tunneling microscope light emission from GaAs

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The electromagnetic enhancement effect in scanning tunneling microscope (STM) light emission from GaAs has been investigated by the finite difference time domain method. We have calculated the intensity of light emitted by the recombination of minority carriers injected from the tip and majority carriers in the sample. The results depend not only on the material and the shape of the tip but also on light polarization. When the tip is tungsten whose dielectric function has a positive real part at 1.5 eV, the p-polarized light intensity depends strongly on the size of the tip and the location of recombination. However, the *s*-polarized light emission depends only weakly on these parameters. If the tip is a perfect metal, the *p*-polarized light intensity becomes a few times stronger than that for the W tip of the same shape. On the other hand, the *s*-polarized light intensity becomes weaker than that for the W tip due to the electromagnetic screening effect of a perfect metal. We conclude that the combination of the W tip and *s*-polarized light detection is suitable for precise measurement of the tip-position dependence of STM light emission properties. A tip with a negative value of the real part of dielectric function is preferable to the W tip, if one does not analyze the tip-position dependence of STM light emission, because STM light emission is enhanced relative to the case of the W tip. [DOI: 10.1063/1.1554473]

I. INTRODUCTION

The recent development of microfabrication technology has made it possible to create nanoscale structures even with an atomic level precision, and the needs for characterization techniques for individual nanostructures are increasing. Scanning tunneling microscope (STM) light emission is an ideal tool for this purpose.[1,2] In this method electrons are injected into a specific nanostructure in the STM image, and the light emitted from that structure is analyzed. Thus one can learn the electronic and optical properties of targeted individual nanostructures.

Spatial resolution is crucial for any local area probing technique. Since the lateral size of the tunneling current of STM is less than 1 nm, atomic scale spatial resolution is achieved for metallic and indirect gap semiconductor samples in STM light emission.[3–5] However, when the sample is a direct gap semiconductor such as GaAs, factors other than the lateral size of the tunneling current play an important role in determining the spatial resolution. STM light emission from a direct gap semiconductor is excited by recombination of minority carriers injected by the tip and majority carriers in the sample. Diffusion of the injected carriers in the sample before electron-hole recombination is one of the major factors that determine the spatial resolution. Alvarado *et al.*[6] and Tsuruoka *et al.*[7] estimated the diffusion length by measuring the STM light intensity as a function of the lateral distance between light emitting quantum structures and the tip position.

Another factor that must affect the spatial resolution but has not been taken into account so far is an electromagnetic enhancement effect of the tip. The electric field generated by an oscillating dipole located in the STM tip–sample gap region is electromagnetically enhanced by the presence of the tip.[8] As a result, STM light emission must be stronger for electron-hole recombination just below the tip than for that away from the gap region. One has to clarify this electromagnetic enhancement effect to properly analyze the STM light emission from a direct gap semiconductor sample.

The conventional STM light emission theories[9,10] are not applicable to the present problem, because they cannot treat radiation from a dipole located at positions other than the center of the STM gap. Very recently Wu and Mills succeeded in avoiding this restriction in their dielectric theory.[11]

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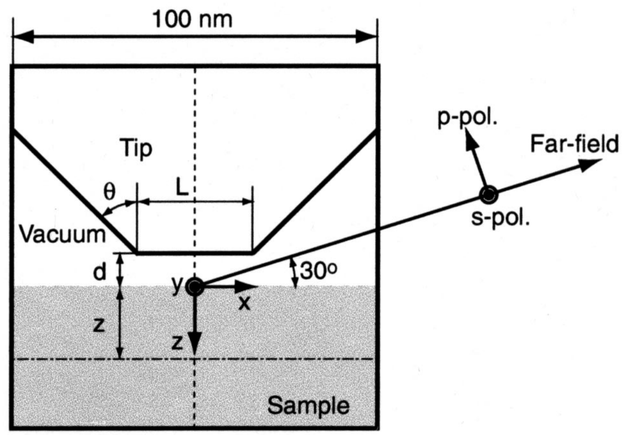

FIG. 1. Cross-sectional view of the STM gap modeled in the present analysis. Electron-hole recombination is represented by a point current source I.

However, we chose not to use the dielectric theory for our analysis. In the dielectric theory of STM light emission including the Wu and Mills theory, a virtual dipole is found from the field induced by a dipole located in the STM gap region in the first step of the calculation, and then the emission intensity is calculated from the far-field radiation of the virtual dipole located on the sample surface. Since the geometrical shape of the tip is not taken into account in the second step, the dielectric theory is not suitable for quantitative analysis of STM light emission intensity.[12] We have calculated the STM light emission intensity as a function of the distance between the tip and the location of electron-hole recombination using the finite difference time domain method (FDTD).[13,14]

II. METHOD

Figure 1 shows the cross-sectional view of the STM gap modeled in the present calculation. The tip shape is specified by angle θ and width L of the tip front. The tip–sample gap distance is denoted by d. We set θ and d equal to 45° and 1 nm, respectively, in the following calculation. The $x-y$ axes and z axis are taken parallel and perpendicular to the sample surface, respectively. The origin of the $x-y-z$ coordinate system lies at the cross point of the sample surface and the symmetrical axis of the tip shown by the vertical dotted line in Fig. 1. The direction of the z axis is taken to be positive in the downward direction as illustrated in Fig. 1. Hence the region $z>0$ corresponds to the interior of the sample.

We modeled the recombination emission of an electron-hole pair in the GaAs sample by a point current source $\mathbf{I}$ (i.e., a current source with an infinitesimally small size):

$$\mathbf{I}(t)=\left[I_x \sin\left(\frac{\Delta E_g}{\hbar}t+\alpha_x\right), I_y \sin\left(\frac{\Delta E_g}{\hbar}t+\alpha_y\right), I_z \sin\left(\frac{\Delta E_g}{\hbar}t+\alpha_z\right)\right], \tag{1}$$

where I_i and α_i are the ith components ($i=x, y, z$) of the amplitude and the phase, respectively; ΔE_g is the band-gap energy of the sample and is fixed at 1.5 eV in the following calculation; $\hbar$ is the Planck constant divided by 2π; t is time. Since the electronic band structure of GaAs is isotropic in the $\mathbf{k}$ space around the band gap, we assumed $I_x=I_y=I_z$. No correlation was assumed between the phases, because the STM light is incoherent, i.e., we set $\langle\alpha_i\alpha_j\rangle=0$ for $i\neq j$. Here $\langle\cdots\rangle$ indicates a statistical average.

The electromagnetic field radiated from the point current source was calculated in a space with the size of 100 nm $\times$100 nm$\times$100 nm by the FDTD method. The calculated space was surrounded by a perfectly matched layer (PML) so that the electromagnetic field arriving at the boundary is not reflected but is perfectly absorbed by PML. Hence one can obtain the electromagnetic field inside the calculated space. The intensity of the light that is radiated in the $x-z$ plane at 30° from the sample surface (i.e., the intensity of the far-field) was calculated by connecting the field obtained by the FDTD method (i.e., the near-field) to the far-field by the standard method in the FDTD analysis.[14] The light with the electric field parallel and perpendicular to the $x-z$ plane are p and s polarized, respectively (see Fig. 1).

We analyzed the electromagnetic enhancement effect for two tip materials. They were tungsten (W) and a perfect metal. W is one of the common materials for the tip. The real part of the dielectric function of W is positive for photon energy of 1.5 eV.[15] The electromagnetic enhancement effect is stronger for the tip with a negative real part than for that with a positive real part like W.[8] This means that the STM light emission efficiency for a tip with a negative real part is higher than that with a positive real part. In order to know how the efficiency is improved by using a tip with a negative real part, we calculated STM light emission for a perfect metal tip whose real part of the dielectric function is negative infinity.

The FDTD method has a limited applicability to electromagnetic problems containing materials with a finite imaginary part of the dielectric function. In the present work, we neglect the imaginary part of the dielectric function of W and GaAs; the dielectric functions of W and GaAs are assumed to be $\varepsilon_{\mathrm{W}}=+4.3$ and $\varepsilon_{\mathrm{GaAs}}=+13.4$, respectively.[15]

III. RESULTS AND DISCUSSION

First we analyze the electromagnetic enhancement effect in the W tip-GaAs sample system. Figures 2(a) and 2(b) show the variation of the p- and s-polarized light intensities, respectively, for current source locations from $z=0$ nm to $z=32$ nm along the vertical dotted line (i.e., the z axis) in Fig. 1. Filled squares, circles, and rectangles correspond to the results for tips with $L=4$, 12, and 24 nm, respectively.

We see from Fig. 2(a) that the p-polarized light intensity depends on both the width L of the tip front and the vertical position z of the current source. While the light intensity for the tip front width $L=4$ nm is greater than that for $L=24$ nm for the vertical position $z=0$, the former decreases faster than the latter with increasing z. As a result the light intensity for z greater than a few nm becomes less for $L=4$ nm than for $L=24$ nm. In contrast to p polarization, the s-polarized light intensity depends weakly on L [see Fig.

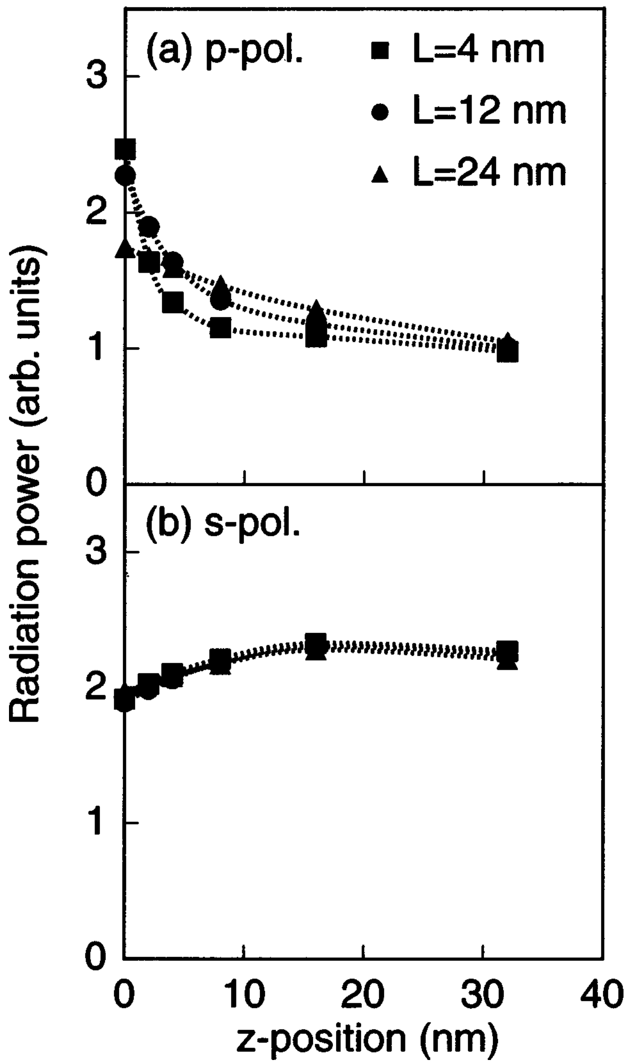

FIG. 2. (a) and (b) show the variation of the *p*- and *s*-polarized light intensities, respectively, for current source locations from $z=0$ nm to $z=32$ nm along the vertical dotted line in Fig. 1. The tip and the sample materials are W and GaAs, respectively. Filled squares, circles, and rectangles correspond to the results for tip widths $L=4$, 12, and 24 nm, respectively. Dotted curves are guides to the eye.

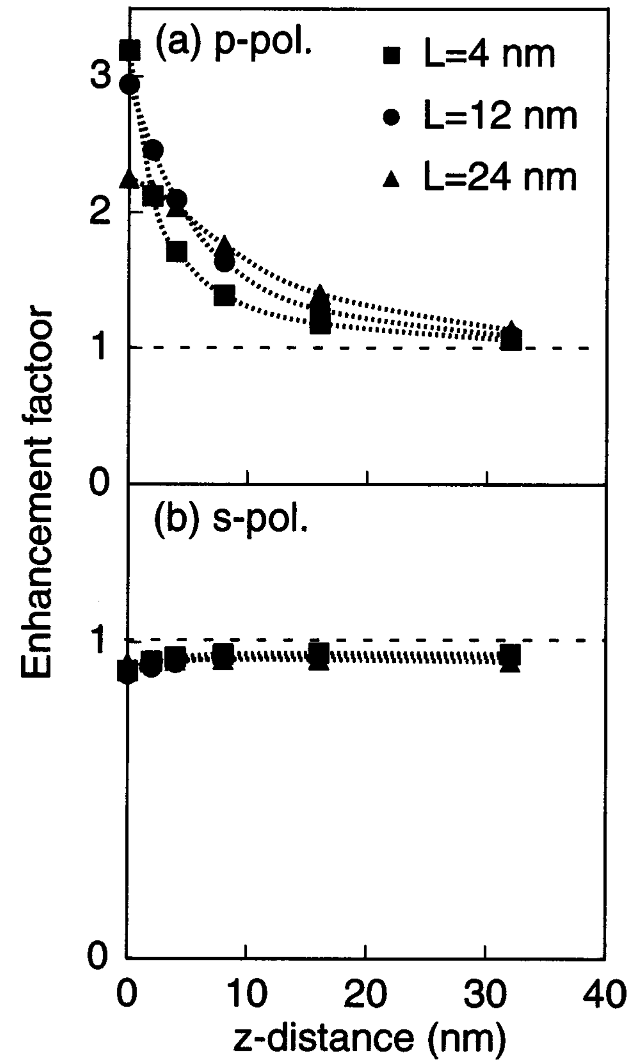

FIG. 3. *z*-position dependence of the enhancement factor of the W tip and GaAs sample system; (a) and (b) correspond to *p*- and *s*-polarized light, respectively. Filled squares, circles, and rectangles are results for tip widths $L=4$, 12, and 24 nm, respectively. Dotted curves are guides to the eye.

2(b)] and monotonically increases with *z*, saturating for $z > 15$ nm. We note that the *s*-polarized light is not weak relative to the *p*-polarized light.

In order to clarify the role of the tip in determining the light emission properties shown in Fig. 2, we calculated the enhancement factor that is defined by the ratio of the light emission intensity with a tip to that without a tip. The enhancement factor greater than unity means that the emission is enhanced by the presence of the tip. Figure 3 shows the *z* dependence of the enhancement factor corresponding to the light intensity in Fig. 2. Figures 2(a) and 2(b) are the results for *p*- and *s*-polarized light, respectively. Filled squares, circles, and rectangles correspond to the results for the tips with $L=4$, 12, and 24 nm, respectively. The enhancement factor for p-polarized light takes the maximum value for the current source position $z=0$ and decreases asymptotically to unity as *z* increases (i.e., the enhancement factor for the current source position far away from the tip is not affected by the presence of the tip). The enhancement factor for *s*-polarized emission is slightly less than unity for the current source position $z=0$ and increases slowly to the asymptotic value of unity for large *z*.

Next, we analyze the variation of the enhancement factor for different current source locations parallel to the sample surface. Figure 4 shows the variation of the enhancement factor for the current source movement from $x=-32$ to 32 nm along the straight line defined by $z=4$ nm and $y=0$ (see the dotted-dashed line in Fig. 1). Figures 4(a) and 4(b) are the results for *p*- and *s*-polarized light, respectively. Filled squares, circles, and triangles show the results for the tips with $L=4$, 12, and 24 nm, respectively. Since the light intensity without the tip depends on the *z* position of the current source but is independent of its *x* and *y* positions, the light intensity corresponding to each enhancement factor in Fig. 3 can be deduced from Fig. 2.

For *p*-polarized light [Fig. 4(a)], the enhancement factor depends strongly on the horizontal position *x* of the current source. When *x* is less than -15 nm (i.e., the current source

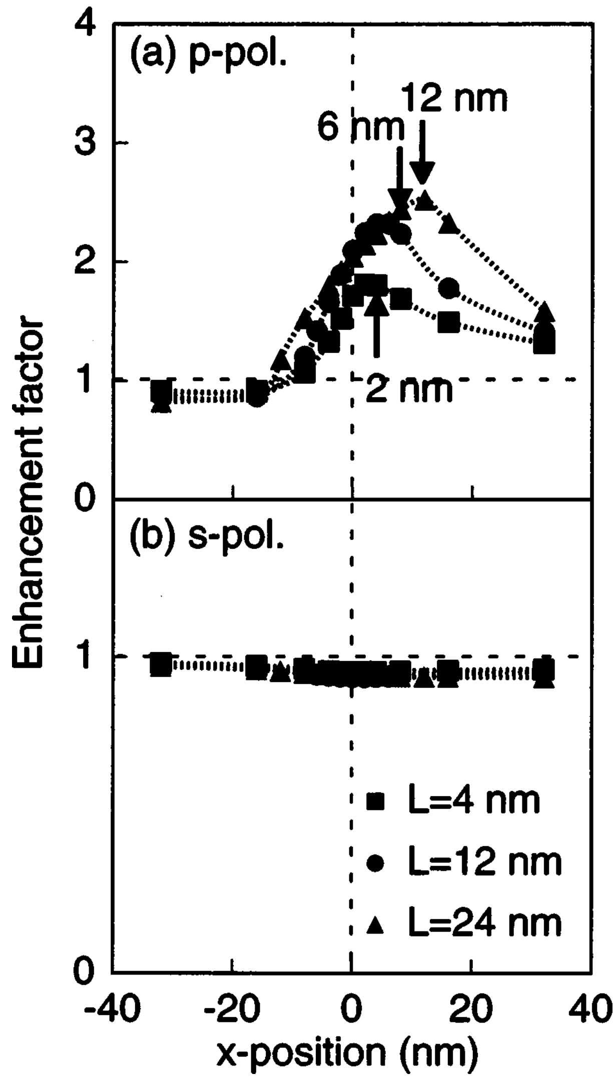

FIG. 4. *x*-position dependence of the enhancement factor of the W tip-GaAs system along the straight line defined by $z=4$ nm and $y=0$: (a) and (b) correspond to *p*- and *s*-polarized light, respectively. Filled squares, circles, and triangles show the results for tip widths $L=4$, 12, and 24 nm, respectively. Dotted curves are guides to the eye.

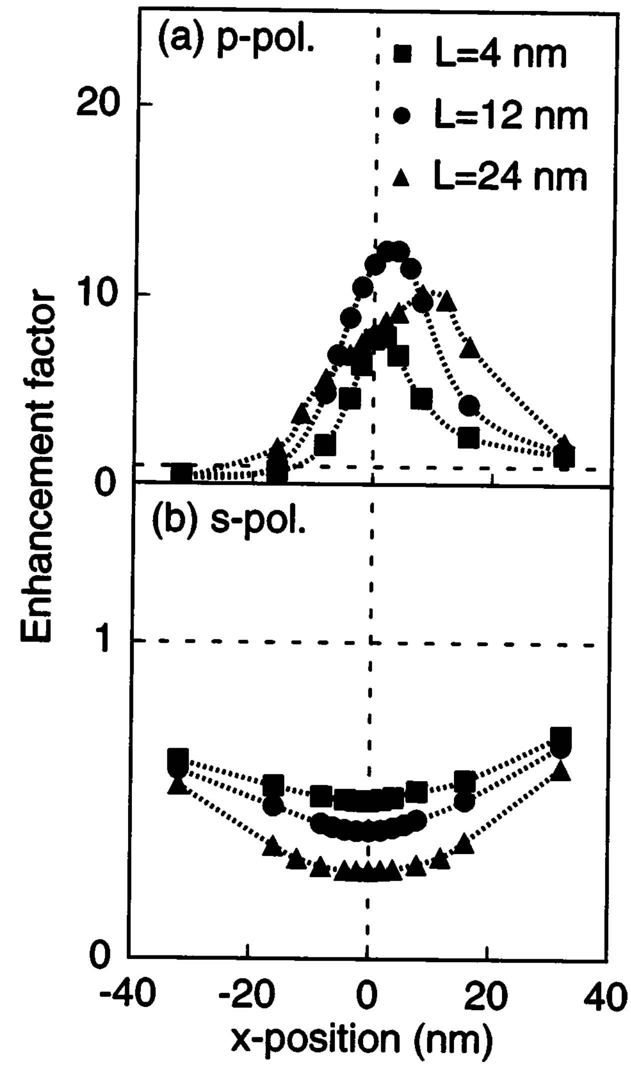

FIG. 5. *x*-position dependence of the enhancement factor for the perfect metal tip-GaAs sample system: (a) and (b) correspond to *p*- and *s*-polarized light, respectively. Filled squares, circles, and triangles show the results for the tip widths $L=4$, 12, and 24 nm, respectively. Dotted curves are guides to the eye.

seen from the observation point is placed beyond the tip), the enhancement factor is less than unity. As the current source approaches the center of the tip $(x=0)$, it increases rapidly. We note that the enhancement factor takes the maximum value at $x=2$, 6, and 12 nm for tip widths $L=4$, 12, and 24 nm, respectively. It takes the maximum value when the current source is placed just below the edge of the tip. Then it decreases to the asymptotic value of unity for large *x*. Figure 4(b) shows the results for *s*-polarized light. In contrast to the case of p polarization, the enhancement factor depends very weakly on *x* and *L*.

Next let us examine the enhancement factor for a perfect metal tip-GaAs sample system. Figure 5 shows the *x*-position dependence of the enhancement factor; the current source is moved from $x=-32$ to $x=32$ nm along the straight line defined by $z=4$ nm and $y=0$. Figures 5(a) and 5(b) are the results for *p*- and *s*-polarized light, respectively. Filled squares, circles, and triangles are the results for tips with $L=4$, 12, and 24 nm, respectively. We see that the maximum value of the enhancement factor for a perfect metal tip is a few times larger than that for the W tip for the same value of *L*. On the other hand, the enhancement factor for *s*-polarized light is less than that for the W tip and depends on *x* and *L*. At the center of the tip $(x=0)$ it takes the minimum value, which becomes smaller with *L*. The origin of this minimum for *s*-polarization light is the screening effect of the perfect metal surface. The components of the current source parallel to the perfect metal surface are strongly damped, because of the electromagnetic screening effect. Hence the *s*-polarized light takes the minimum intensity at the center of the tip.

As seen from Figs. 4 and 5, the *x*-position dependence of the enhancement factor for *p*-polarized light is asymmetrical with respect to the center of the tip $(x=0)$. We will now demonstrate that this asymmetry is characteristic of the STM light emission from a GaAs sample, i.e., characteristic of a direct gap semiconductor sample and not that of the specific tip shape. For this purpose we have calculated the *x*-position dependence of the enhancement factor of the W tip-perfect

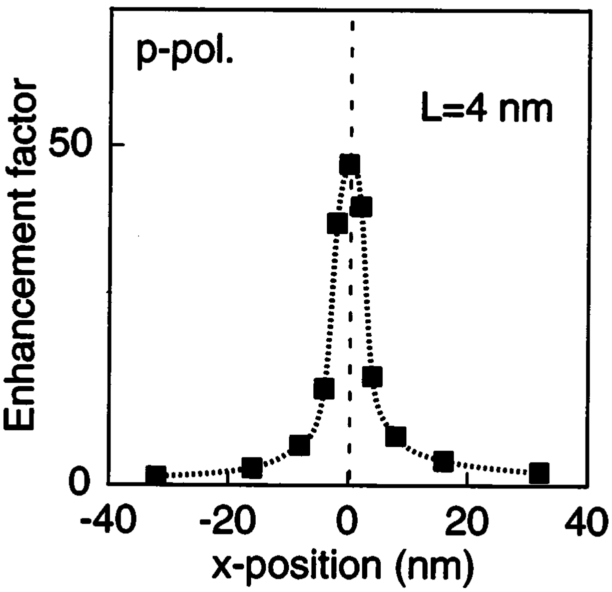

FIG. 6. *x*-position dependence of the enhancement factor of the W tip-perfect metal sample for *p*-ploarized light. Here the tip width *L* is fixed at 4 nm. Dotted curve is a guide to the eye.

metallic sample system using the same tip shape. We note that the STM light emission from a metallic sample is not excited by electron-hole recombination. In use of a metallic sample, light emission is radiated by localized surface plasmons confined in the gap between the tip and sample. Thus, we place the current source in the vacuum above the sample surface. In this case, as already pointed out, the components of the current source parallel to the surface are strongly damped. Hence, we set $I_x = I_y = 0$ here.

Figure 6 shows the variation of the enhancement factor with a movement of the current source from $x = -32$ to 32 nm along the straight line defined by $z = -0.5\,\mathrm{nm}$ and $y = 0$ for *p*-polarized light. Since we set $I_x = I_y = 0$, no s-polarized light is emitted. The tip front width *L* was fixed at 4 nm. In contrast to the GaAs sample case, the enhancement factor takes the maximum value for $x = 0$, and its shape is almost symmetrical with respect to the center of the tip. Hence we can conclude that the asymmetry seen in Figs. 4 and 5 is characteristic of the STM light emission from a GaAs sample or more generally from a direct gap semiconductor as opposed to a metallic sample. This difference probably arises from the fact that for a metallic sample the current source is located in the vacuum above the sample surface and not inside the sample.

As already pointed out, the tunneling current of STM is focused to an atomic size in the lateral direction. Hence, the STM is an ideal tool to excite light emission from individual quantum semiconductor structures. We found that the enhancement factor for *p*-polarized light depends strongly on the location where electron-hole recombination takes place. Thus one must take into account the electromagnetic enhancement effect in analyzing the tip-position dependence of the STM light emission characteristics. For example, if *p*-polarized STM light was measured to determine the diffusion length of minority carriers, one must isolate the electromagnetic enhancement effect from the observed results to obtain its precise value. Figure 4(b) shows that *s*-polarized light emission measurements are preferable for precise determination of the diffusion length, because no correction for the experimental result is required.

STM light emission is basically weak, because the tunneling current is limited to a nanoampere level to avoid sample damage. If one wants to observe STM light emission from an isolated quantum semiconductor structure but does not intend to analyze the tip-position dependence of the emission characteristics, a tip with a negative value of the real part of dielectric function is suitable, because the STM light is enhanced more strongly than for the case of a W tip.

IV. CONCLUSION

The electromagnetic enhancement effect in STM light emission from GaAs has been analyzed for W and perfect metal tips by the FDTD method. When the tip material is W, the *p*-polarized light intensity depends strongly on the size of the tip and the location of recombination with respect to the tip, but the *s*-polarized light emission depends very weakly on these parameters. For a perfect metal tip the *p*-polarized light intensity is a few times stronger than that for the W tip with the same shape. However, the *s*-polarized light intensity is weaker than that for the W tip, due to the electromagnetic screening effect of the tip. We found that the combination of a W tip and *s*-polarization light detection is best for a precise measurement of the tip-position dependence of STM light emission characteristics. A tip with a negative value of the real part of dielectric function is more preferable than a W tip when one does not analyze the position dependence of the STM light emission characteristics.

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