Effect of Ionized Impurity on the Sequential Tunneling Transfer of an Electron through a Quantum Disk

Mitsuru Ishida, Masahito Yamaguchi and Nobuhiko Sawaki

Department of Electronics, Nagoya University, Chikusa-ku, Nagoya 464-8603, Japan
Phone & FAX : +81-52-789-3319,
E-mail: m-isida@nuee.nagoya-u.ac.jp

The motion of a wavepacket injected into a two dimensional GaAs disk was analysed by solving the time dependent Schrödinger equation with finite element method. It was found that the presence of an ionized impurity varies the motion of the wavepacket in the disk which results in a modification of the tunneling transfer probability to an electrode connected to the disk. The transfer probability as a function of the position of an impurity is discussed in terms of the probability amplitude of electrons in front of the potential barrier.

1. Introduction

A typical single electron tunneling device consists of a quantum dot/disk and two electrodes connected via thin potential barriers [1]. The injection/ejection of an electron into/out of the dot/disk is due mainly to tunneling transition, which is most likely to occur through a point where the potential barrier thickness is the thinnest. If the device is of planar structure and size of the disk is on the order of the electron wave length, or if it is mesoscopic, the motion of an electron injected into the disk is to be treated in terms a wave packet which shows non-uniform distribution of the probability amplitude [2]. Since the tunneling transfer probability out of the disk into another electrode might be influenced by the probability amplitude in the disk established near the point where the potential barrier thickness is the thinnest, it would be subject to the two dimensional motion of the wave packet in the disk.

If there is an ionized impurity in or near the disk, the motion of the wave packet will be modified by the presence of attractive/repulsive potential, and the probability amplitude in front of the tunneling barrier will be varied to modify the tunneling transfer probability. In this paper, we will demonstrate important role of an ionized impurity in determining the sequential tunneling probability and show that it depends strongly on the position where the impurity is sitting.

2. Model Structure and Numerical Method

A model system under study is shown in Fig.1(a); a disk of 40 nm diameter is connected to two electrodes along x-axis. To simplify the analyses the shape of the electrode is assumed to be a semi-circle at the contact and the thickness of the tunneling barrier is 2 nm. As physical parameters, we assumed a GaAs/AlGaAs 2DEG system.

At t=0, a Gaussian wave packet of the following form was given at (x_0, y_0) within the left hand side electrode(I);

$$\phi(x, y, t=0) = \frac{1}{\sqrt{\pi\sigma^2}} e^{ik_x x - \frac{(x-x_0)^2+(y-y_0)^2}{2\sigma^2}}, \tag{1}$$

where σ represents the initial size of the wave packet, and k_x is the momentum determined by the kinetic energy along x-axis ($E_x = \frac{\hbar^2 k_x^2}{2m^*}$). In the following, results are obtained with the parameters; $(x_0, y_0) = (-22, 20)$, σ=7nm, E_x = 20meV, which are rather arbitrally but selected to minimize the effect of the finite size of the electrodes on the results. The evolution of the wave packet in the x-y plane is expressed by the time dependent two dimensional Schrödinger equation of the form;

$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\phi + (V + V_I)\phi = i\hbar\frac{\partial}{\partial t}\phi, \tag{2}$$

where the confinement potential V is given by

$$V = \begin{cases} 0 \quad \text{eV,} & \text{within the electrodes and disk} \\ 0.3 \quad \text{eV,} & \text{otherwise,} \end{cases} \tag{3}$$

and the potential for an ionized impurity sitting at (x_i, y_j) is

$$V_I = \frac{\pm 0.109 \times 10^{-9}}{\sqrt{(x-x_i)^2 + (y-y_j)^2}} [\text{eV}]. \tag{4}$$

In Eq.(4) the sign corresponds to negative or positive ion, the dielectric constant for bulk GaAs is adopted, and the

0-7803-4369-7/98 $10.00 ©1998 IEEE

screening effect was neglected for the sake of simplicity. The confining potential V was assumed to be rigid and the variation due to injection of electrons is neglected. The solution was obtained by solving Eq.(2) with the finite element method. The details of the method and general results were published elsewhere [2].

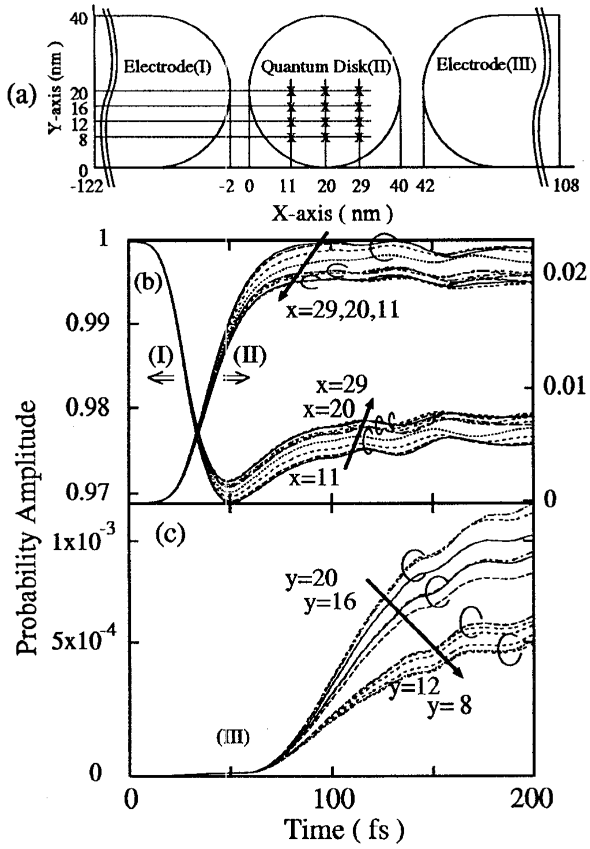

Fig.1 (a)Model structure used in the simulation. Twelve positions of an impurity are shown by crosses. (b)(c)Integrated probability amplitude as a function of time in each region with a positive ion in quantum disk. In electrode(I) and disk(II), curves can be grouped by X-axis coordinate of an ion, while in electrode(III), they are grouped by Y-axis coordinate.

3. Numerical Results

In the previous report [2], it was shown that when the wave packet attacks the potential barrier between the left hand side electrode (I) and the disk (II) finite probability amplitude appears by tunneling effect at the left hand end of the circular disk, which propagates gradually to the right hand side within the disk. In the time duration of t=70 ~ 100 fs, reflection of the wave packet at the right hand end of the disk promotes the formation of the eigen modes within the disk and generates tunneling transfer into the right hand side electrode (III). Thus in the present system, we have two tunneling processes which occur sequentially. In this paper, variation of the probability amplitude achieved in the right hand side electrode (III) is studied by putting an ionized impurity in the disk (II). We tested twelve positions shown in Fig. 1(a).

Figures 1(b) and (c) show typical results obtained putting a positive ion (attractive potential), where the integrated probability amplitude in each region (electrodes (I), (III) and quantum disk (II)) is displayed as a function of time. Due to the tunneling transfer through the first barrier, the probability amplitude in the left hand side electrode (I) decreases, which is accompanied by the increase of the probability amplitude in the disk (II). The increase of the probability amplitude in the right hand side electrode (III) shows a delay due to the propagation of the wave packet in the disk. In this particular example, the tunneling transfer through the first potential barrier is almost completed by 100 fs, while we need more time for that through the second barrier.

In Figs. 1(b) and (c), the curves are sensitive to the position of the impurity. Remarkable fact is that the tunneling process through the first barrier is sensitive to the x-axis coordinate of the impurity, while that for the second barrier is more sensitive to the y-axis coordinate. For the first barrier tunneling, the transfer probability is more enhanced by putting the impurity near the barrier. This is simply because the potential barrier height is lowered by putting the positive ion near the barrier. For the second barrier tunneling process, on the other hand, the transfer probability is more enhanced by putting the impurity in the disk near the center line ($y = 20$) of the model system, of which reason is not obvious.

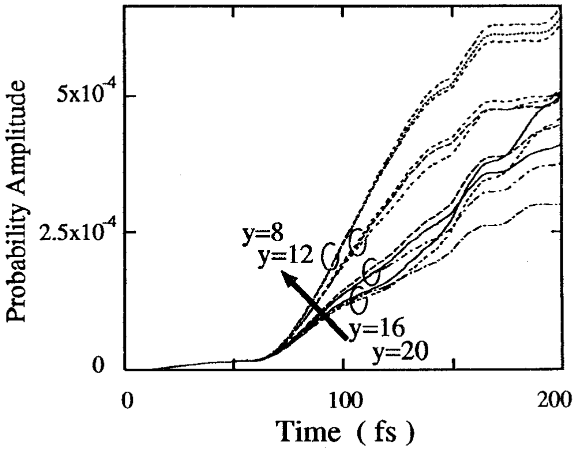

Fig.2 Integrated probability amplitude as a function of time in electrode (III) with a negative ion in quantum disk.

In case we put a negative impurity in quantum disk, injection of probability amplitude in quantum disk was suppressed by the increase of the effective potential barrier height, and similar results as of Figs.1(b) and (c) were obtained except that the dependence of x-axis and y-axis coordinate was just the contrary (Fig. 2).

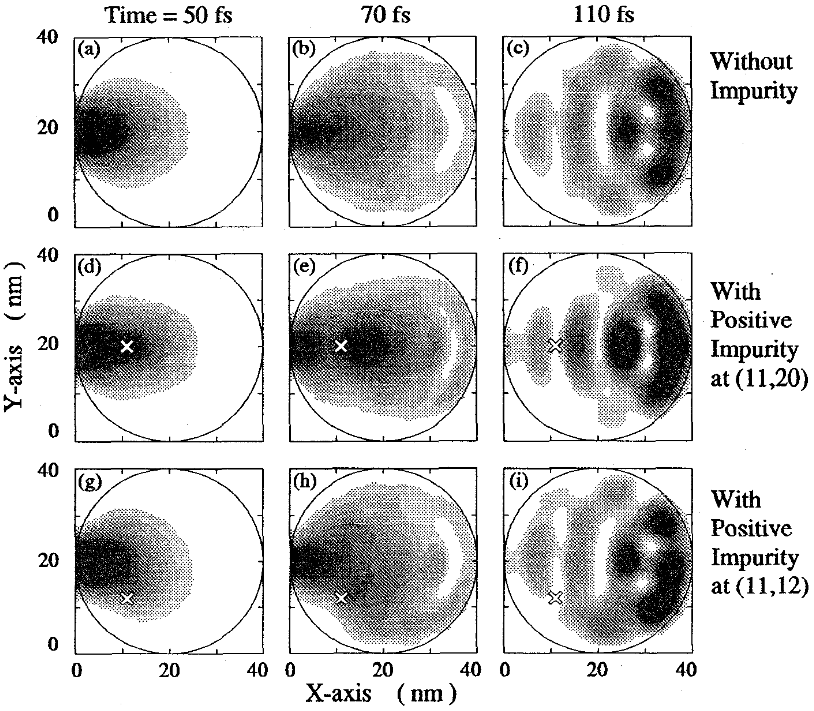

Fig.3 Evolution of the probability amplitude in quantum disk with/without positive ionized impurity. (The impurity was put at a point indicated by the cross.)

In order to find the cause of these observation, the evolution of the mode structure or the distribution of the probability amplitude within the disk were studied in detail. Figure 3 depicts typical results obtained for a positive impurity at t=50, 70 and 110 fs. For the sake of comparison, results for a case with no impurity are also displayed. Obviously, by putting a positive impurity the probability amplitude in the disk is enhanced. If the y-axis coordinate is not on the center line (Fig.3(g)), the oblique propagation of the wave packet is obvious. At t=70 fs (Fig.3(e)), we get more probability amplitude in front of the second tunneling barrier (that is at the right hand end of the figure), which is suppressed a little bit by varying the y-axis coordinate (Fig.3(h)). At t=110 fs, the difference is more enhanced, i.e., the positive impurity enhances the probability amplitude in front of the second potential barrier where the thickness is the thinnest, and it is modified by replacing the y-axis coordinate of the impurity. In conclusion we have found that the additional potential due to the ionized impurity modifies the manner of propagation of the wave packet as well the distribution of the probability amplitude within the disk.

4. On the Mechanism of the Modification of Tunneling Transfer

In the following we will discuss in detail on the y-axis coordinated dependence of the tunneling transfer through the second barrier. Figure 3 suggested that the electron probability amplitude in front of the second tunneling barrier determines the probability amplitude achieved in the right hand side electrode. In order to understand this point in more detail, in Fig.4(a) we plotted magnitude of the probability amplitude at the right hand end of the disk P(x=40,y=20) as a function of time. Figure 4(b) shows the integrated value. The appearance of a peak in Fig.4(a) is attributed to the back and forth movement of the wave packet in the disk. It is notable that the curves are very sensitive to the y-axis coordinate of the impurity. Surprisingly, the curvatures shown in Fig.4(b) are quite similar to those shown in Fig.1(c). Moreover, the y-axis dependence is almost the same. Slight disagreement might be screened by considering finite spread of the tunneling path around the point at which the potential barrier thickness is the thinnest. This proves that the electron probability amplitude achieved in the electrode (III) is determined by the local probability amplitude of electrons in front of the potential barrier in the disk.

Our second test was how the mode structure is varied by the presence of an ionized impurity, i.e., what is the difference of the electron probability amplitude raised by putting an impurity to cause the y-axis dependence of the probability amplitude in front of the second tunneling barrier. Figures 5 show typical results obtained at t=70 fs. If the impurity is near the left hand side potential barrier (Fig.5(a)), we see strong enhancement of the probability amplitude propagating toward the right

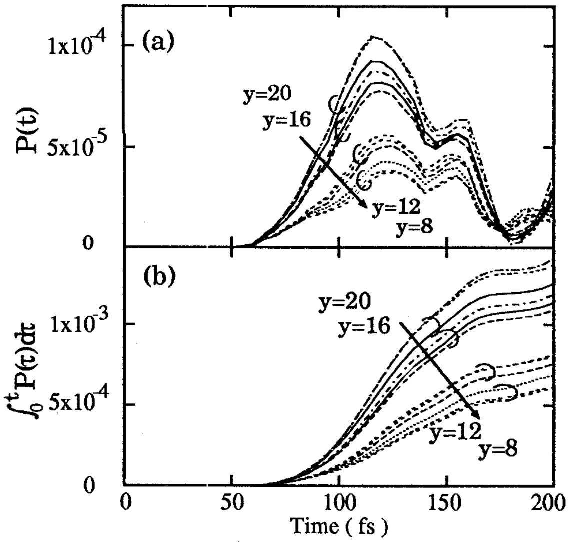

Fig.4 (a) The probability amplitude mesured at (x=40,y=20). (b) Time integrated value of the probability amplitude mesured at (x=40,y=20).

hand side potential barrier, along with negative fringe developed perpendicular to the propagation. This is attributed to the self-interference effect of the wave packet which is originated from the attractive Coulomb potential [2,3]. If we put an impurity near the right hand side potential barrier (Fig.5(c)), on the other hand, interaction with the ionized impurity made additional mode which is independent of the original confinig potential. Any way, the probability amplitude in front of the second tunneling barrier is enhanced. By moving the impurity along y-axis(Fig.5(d)), the high probability amplitude part is pulled by the attractive potential, which in turn modify the probability amplitude at (x=40,y=20). These observation shows the origin of the y-axis coordinate dependence of the probability amplitude achieved in the right hand side electrode (III).

Finally we might raise a naive question on the conclusion. We may decompose the wave packet into a combination of plane waves with different energies and different phases. If we apply elemental tunneling theory for each component, we might have different tunneling probabilities for each component. If we do not consider any dissipation or phase breaking mechanism in the processes, we might have a total transfer probability which is just given by reconstructing the transmitted plane waves beyond the potential barrier or in the electrode (III). In the present study, we are simply solving the Schrödinger equation and do not take into account of any dissipation processes. So we might get tunneling probability which should be determined by all the plane waves or the total modes in the whole area of the disk. But results presented above suggested that the final result is determined by the probability amplitude (electron density) just in front of the tunneling barrier. We do not understand straight forwardly why the information far from the barrier could be omitted in the whole process, which will be a subject of further study.

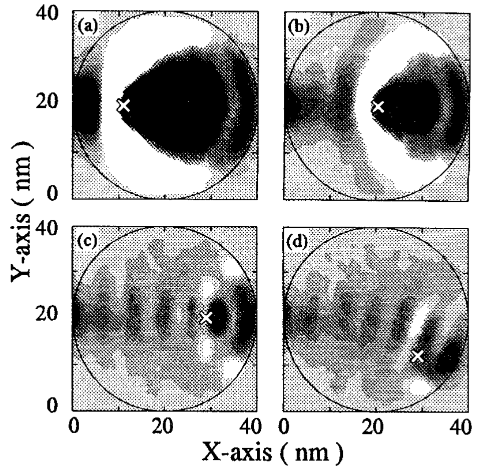

Fig.5 Difference in the probability amplitude raised by putting a positive impurity(at cross).

5. Summary

The time dependent Schrödinger equation has been solved to study the effect of an ionized impurity on tunneling phenomena in a model system which consists of quantum disk and two electrodes connected via thin tunneling barrier. It was found that an impurity modifies the propagation of an wave packet in the disk and the subsequent tunneling probability depending on the position of the ionized impurity. The magnitude of probability amplitude at a point where the barrier thickness is the thinnest almost determines the tunneling probability.

Acknowledgments

This work was partly supported by the Grant-in-Aid from the Ministry of Education, Science, Culture and Sports of Japan.

References

1. L.P. Kouwenhoven et al : *Nanostructures and Quantum Effects,* eds. H. Sakaki and H. Noge: (Springer-Verlag, 1994) p95.
2. M. Ishida, M. Yamaguchi and N. Sawaki: 1998 Intern. Symp. Formation, Physics and Device Appri-cation of Quantum Dot Structures, Hokkaido, Sapporo, 1998, We2-3., Submitted to Jpn.J.Appl.Phys.
3. U. Sivan, M. Heiblum, C.P. Umbach and H. Shtrikman: Phys. Rev. **B41** (1990) 7937.