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Time-Evolved Simulation of a Two-Dimensional Electron Wave Packet through a Quantum Slit

Akira Endoh, Shigehiko Sasa, Hiroshi Arimoto, Shunichi Muto, and Toshio Fujii

Fujitsu Laboratories Ltd.
10-1 Morinosato-Wakamiya, Atsugi, 243-01, Japan

We performed time-evolved numerical simulations of a two-dimensional electron wave packet through single and double slits by the finite difference method, simulating electron diffraction and quantum interference phenomena. For a single slit, the starting point of electron diffraction is at the center of the slit entrance. For a double slit, the starting point of quantum interference is at the center between the two slit exits. For the single slit, we found a delay in the motion of subpeaks due to quantization inside the slit.

1. Introduction

Recent developments in crystal growth and nanometer-scale processing techniques have enabled us to fabricate nanostructures in which the electrons show a wave nature such as quantum interference effects. A basic understanding of the physical properties of the electron wave in these structures is required. We performed time-evolved numerical simulations of a two-dimensional electron wave packet by the finite difference method. This method can be applied to systems which can not be solved analytically. Cahay *et al.* used a similar simulation technique and confirmed the formation of diffraction subpeaks in an electron wave passing through a single slit[1]. In this work, we performed numerical simulations of an electron wave packet through single and double quantum slits. We confirmed the formation of interference subpeaks in an electron wave passing through the double slit.

2. Numerical Simulation

In numerical simulations, we used a difference equation of the time-dependent Schrödinger equation,

$$\begin{aligned}\psi(x,y,t+\Delta t) = {} & \psi(x,y,t-\Delta t) \\ & +(i\hbar/m^*)\,[\Delta t/(\Delta r)^2] \\ & [\psi(x+\Delta r,y,t)+\psi(x-\Delta r,y,t) \\ & +\psi(x,y+\Delta r,t)+\psi(x,y-\Delta r,t)-4\psi(x,y,t)] \\ & -(i2\Delta t/\hbar)\,V(x,y)\,\psi(x,y,t), \end{aligned} \quad (1)$$

where ψ is a wave function, $\hbar$ the Planck constant divided by 2π, m^* the effective electron mass, i the imaginary unit, Δt the time step, Δr the grid step, and V potential energy.

As an initial wave function, a two-dimensional Gaussian wave packet was used,

$$\begin{aligned}&\psi(x,y,t=0) \\ &= (\alpha/\pi)^{1/2} \exp[i(k_x x+k_y y)-\alpha(x^2+y^2)/2], \end{aligned} \quad (2)$$

where α is a parameter determining the Gaussian distribution, and k_x (k_y) the wave number on the x axis (y axis), calculated from the incident energy of the electron wave packet. In the present simulations, wave numbers k_x and k_y were made equal. Therefore, an initial electron wave packet is propagated at an angle of 45°. The effective electron mass m^* was assumed to be 0.068 m_e(m_e : electron rest mass), corresponding to GaAs. The energy of the potential barrier is 0.25 eV, and the profile varies as a step function. The square plane was 600 nm x 600 nm. The grid step Δr was 2 nm on

both x and y axes. The time step Δt was 0.2 fs.

3. Results and Discussion

a) Single Slit

Figure 1 shows a bird's eye view of time evolution of the probability density of an electron wave packet $|\psi(x,y,t)|^2$ through a single slit 50 nm wide and a potential barrier 10 nm thick. A schematic profile of the potential barrier is shown in the figure at t=0. The electron wave packet starts to impinge on the potential barrier wall at about t=0.2 ps. At t=0.4 ps, the transmitted wave is split into several components, i.e., the electron diffraction phenomenon is simulated.

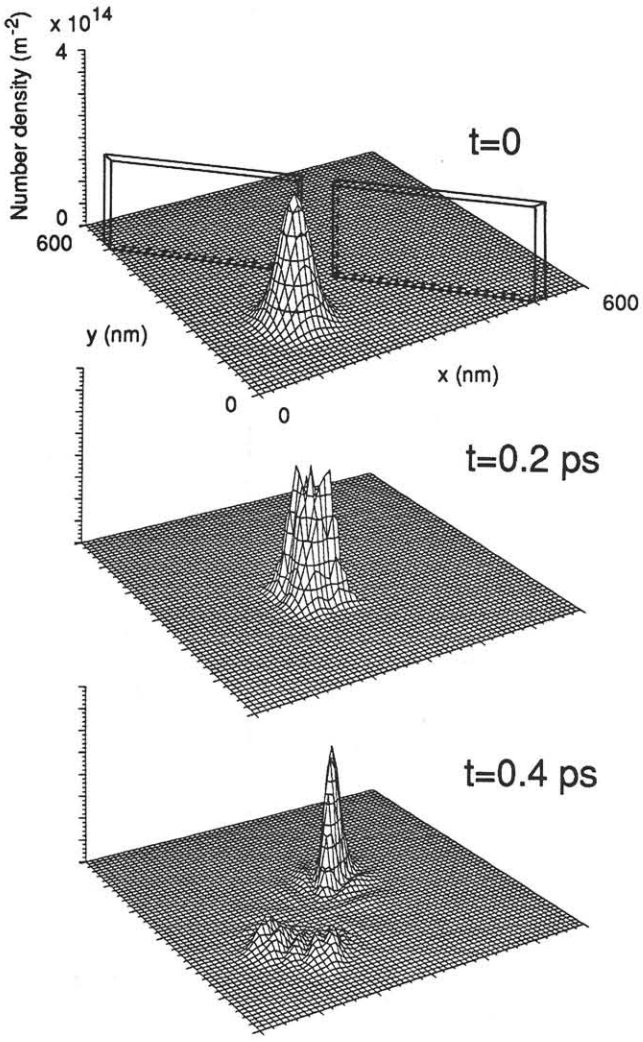

Fig. 1 Bird's eye views of the time evolution of the probability density of an electron wave packet for a slit 50 nm wide and a potential barrier 10 nm thick.

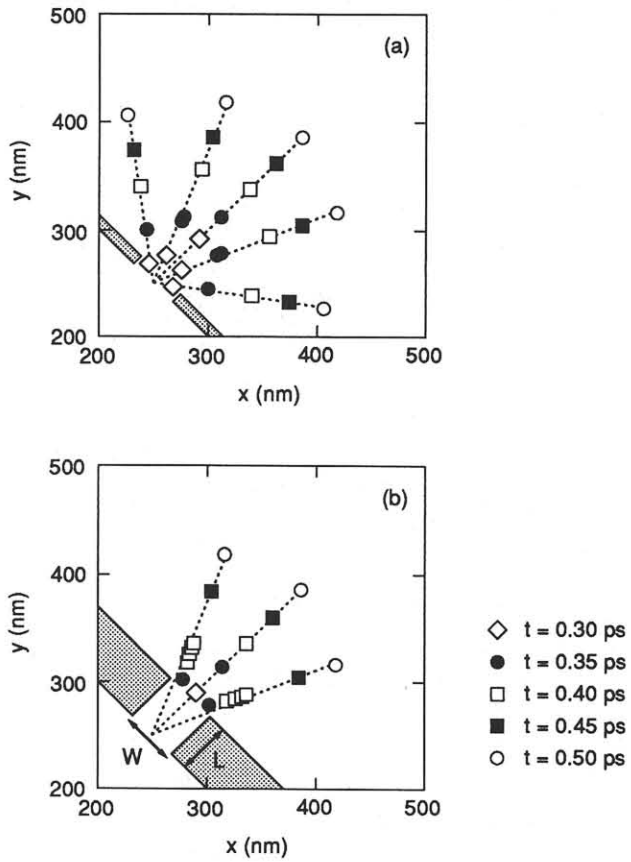

Fig. 2 Traces of peak positions of the wave transmitted through a single slit.
(a) W=50 nm, L=10 nm
(b) W=50 nm, L=50 nm
Initial wave packet conditions are the same for both (a) and (b).

For a better understanding of the motion of transmitted waves, we studied the motion of peaks at chosen time steps. Figure 2 shows the traces of the peak positions of the transmitted wave. The dotted lines connecting the peak of each component show that the starting point of electron diffraction is at the center of the slit entrance. With an increase in the potential barrier thickness L, the outermost subpeaks disappear, but inner subpeaks are unchanged. At a longer L, components with high diffraction angles may be reflected by the inside wall of the slit. Diffracted subpeaks delay due to quantization inside the slit. By calculating group velocities of transmitted waves, we found that the wave numbers in the vertical direction are quantized. Therefore, the diffraction angles are determined by slit width W. The number of allowed diffracted components is determined by

potential barrier thickness L. Our calculation also showed that the number of diffracted subpeaks and diffraction angles are independent of the initial shape of the electron wave packet.

b) Double Slit

Figure 3 shows the $|\psi(x,y,t)|^2$ at t=0.4 ps, just after passing through a double slit. Each slit was 10 nm wide, spaced at 40 nm, with a potential barrier 10 nm thick. For a single slit 10 nm wide, only one component can be transmitted straight through the slit. Therefore, the subpeaks of the transmitted wave in Fig. 3 are regarded as formed by quantum interference effects.

Figure 4 shows the traces of peak positions of the interference wave plotted similarly to Fig. 2. Dotted lines show that the starting point of quantum interference is at the center between the two slit exits. Therefore, the number of interference components is the same for (a) and (b), in contrast to Fig. 2. The peak positions at the same time step lie the same distance from the starting point, which means no delay time for a double slit.

The difference between diffraction and interference can be interpreted as follows: Since diffraction depends strongly on the quantum levels formed in a slit, the entrance of the slit where electron waves are quantized plays a dominant role. Interference is caused by the overlapping of several electron waves.

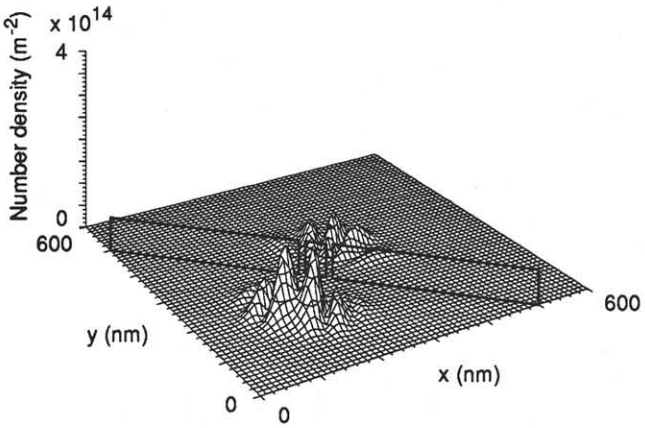

Fig. 3 Bird's eye view of the probability density of electron wave packet at t=0.4 ps for slits each 10 nm wide, 40 nm apart, and a potential barrier 10 nm thick.

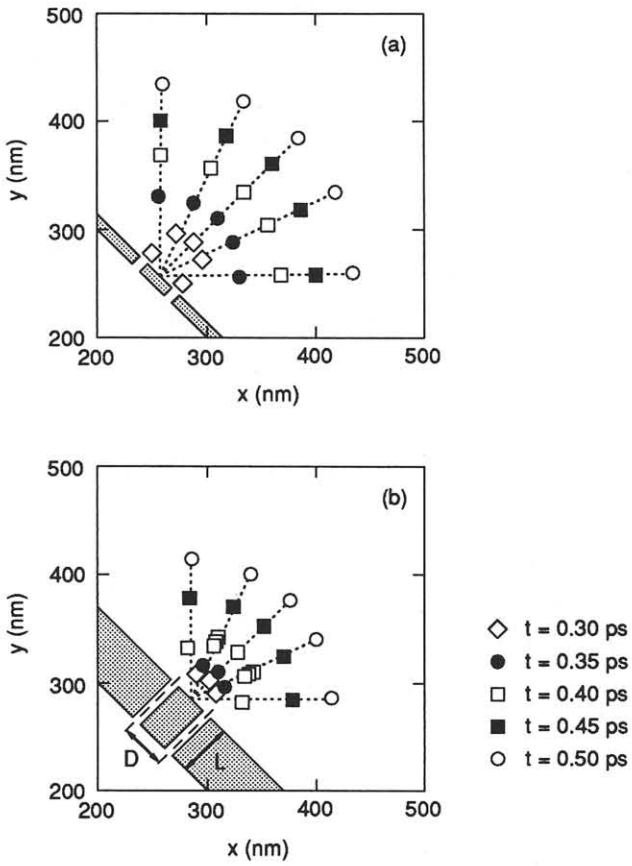

Fig. 4 Traces of peak positions of the wave transmitted through a double slit.
(a) W=10 nm, D=40 nm, L=10 nm
(b) W=10 nm, D=40 nm, L=50 nm
Initial wave packet conditions are the same as for a single slit.

Therefore, slit exits determine the shape of interference wave peaks.

In conclusion, we performed time-evolved numerical simulations of an electron wave packet through single and double slits, simulating the wave nature of electrons, e.g., diffraction and interference effects. The method is a powerful tool in simulating the wave nature of electrons.

Acknowledgments

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Reference

1) M. Cahay, J. P. Kreskovsky, and H. L. Grubin, Solid-State Electronics, 32, 1185 (1989).