Quantum interference depression in thin metal films with ridged surface

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Thanks to recent development of nanoelectronics, devices such as resonant tunneling diodes and transistors, super-lattices, quantum wells, and others, based on wave properties of electrons are fabricated. We discuss what happens when low dimensional regular indents are fabricated on the surface of a thin metal film. Using corresponding theoretical methods, we study the free electron inside a potential-energy box with ridged wall and compare the results to the case with plane walls. It was shown that, ridged geometry of the wall leads to Quantum Interference Depression (QID), or reduction of the density of quantum states for the electron. Results obtained for the potential-energy box were extrapolated to the low-dimensional metals (thin metal films). QID leads to increase of the Fermi level and corresponding reduction of the work function. Experimental possibility of fabricating such indents on the surface of a thin metal film was studied.

Assume a rectangular potential-energy box, with one of the walls modified as shown in Fig.1. The indents on the wall have the shape of strips of depth of a and width w. We name the box shown on Fig.1 as Ridged Potential-Energy Box (RPEB) to distinguish it from the ordinary Potential-Energy Box (PEB). The time-independent Schrödinger equation for an electron wave function inside the RPEB can be rewritten in the form of Helmholtz equation

$$(\nabla^2 + k^2)\,\Psi=0, \tag{1}$$

where Ψ is wave function and k is wave vector. For the case $a/2L_x \ll 1$ we use the volume perturbation method to solve the Helmholtz equation [1]. The big rectangular box is regarded as the Main Volume (MV) and the total volume of strips is regarded as the Additional Volume (AV) (Fig.2). Let $\Psi_m(x, y, z)$ be the wave function of electron in the MV and $\Psi_a(x, y, z)$ in the AV. The matching conditions will be $\Psi_m= \Psi_a$, and an equation of partial derivatives of Ψ from two sides, for all points of the connection area. Analysis show that maximized spectrum of wave vector k in RPEB is following:

$$k^x_p=\pi p/a, \quad k^y_q= \pi q/w, \quad k^z_i=\pi i/L_z. \tag{2}$$

Here, k^x_p, k^y_q and k^z_i are x, y, z components of wave vectors and p, q, i=1, 2, 3… Eq. 2 indicates the dramatic reduction in spectrum density of x and y components of wave vector, compared to spectrum density of PEB ($k^x_n= \pi n/L_x$, $k^y_j =\pi j/L_y$, $k^z_i=\pi i/L_z$).

For the case of larger $a/2L_x$, different method was used. The general solution of Eq.1 in such a complicated geometry exhibits several problems. A complicated surface shape does not allow finding an orthogonal coordinate system that will permit separating of variables. However, there are methods that allow one to obtain a dispersion equation and to calculate the wave vector. We used the method of solving Eq.1 inside the corrugated waveguides [1]. Method is based on finding the roots of transcendental equation. We found numerical solutions for high $a/2L_x$ and obtained the same result, namely the dramatic reduction of the spectrum density for RPEB relative to PEB.

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To extrapolate results obtained for RPEB to low-dimensional metal we use a quantum model of free electrons. For T>0, there are two types of free electrons inside the Fermi gas. Electrons with $k \approx k_F$ interact with their environment and define the transport properties of metals. Electrons with $k \ll k_F$ do not interact with the environment, because all quantum states nearby are already occupied by other electrons. Such electrons are ballistic and have formally infinite mean free path. This feature allows us to regard them as planar waves, traveling between the walls of the low-dimensional metal. Further, we will concentrate on such ballistic electrons. Once we work with electrons having infinite (or very long) mean free paths, we can regard the low-dimensional metal as a potential-energy box and extrapolate our calculations to it [2]. We found that in metal films with ridged surface, the volume of elementary cell in k space increase because of QID. Electrical neutrality requires that the same (normalized to volume) number of electrons occupy separate quantum levels. Therefore Fermi sphere expands and Fermi vector increase to the value $k_R = k_F\, [L_y(L_x + a/2)/(aw)]^{1/3}$. Here k_R is Fermi vector in ridged film and k_F is Fermi vector in plain film. For Fermi energy we find

$$E_R = E_F + \alpha_n E_F \left\{ [L_y(L_x + a/2)/(aw)]^{2/3} - 1 \right\}, \tag{3}$$

where E_R and E_F are Fermi energy of ridged and plain films. In practice, electron de Broglie wave will scatter on nonregularityes such as grain boundaries inside the film and roughness on the surface. This reduces QID waveband. Corresponding reduction constant $0<\alpha_n<1$ is introduced in Eq.3 to adjust it to particular set of nonregularityes. For ideal single crystal with zero surface roughness $\alpha_n=1$.

We show that, in the low-dimensional metal films with ridged surface, QID effect reduce the energy spectrum density for electrons and increase the Fermi energy. Using volume perturbation method we calculate approximate analytical expression for the relative increase of the Fermi energy. Our resent experiments show reduction of work function in Au, Nb and SiO_2 thin films with ridged surface [3]. Experimental results are in qualitative agreement with Eq.3.

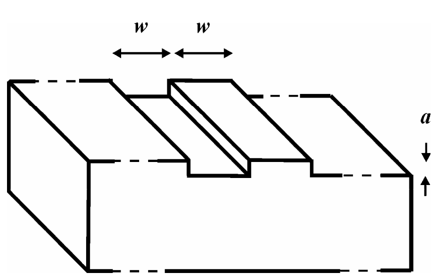

Fig.1 3D view of RPEB.

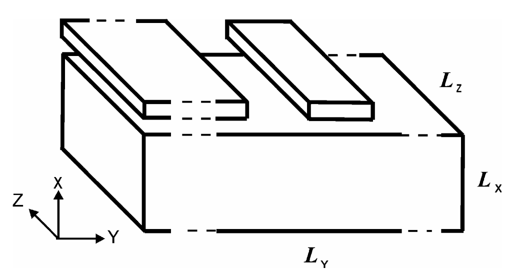

Fig.2 Box with ridged wall, divided it two.

[1] V.M. Sedykh, *Waveguides With Cross Section of Complicated Shape* (Kharkhov Univ. press, 1979), p.16.
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[3] A. Tavkhelidze et. al , *J. Vac. Sci. Technol.* B **24**, 1413 (2006).