

Influence of Surface Roughness on the Fermi Energy Oscillations of Metal Nanofilms

A.V. Korotun^{1,*}, I.M. Titov²

¹ Zaporizhzhya National Technical University, 64, Gogol St., 69063 Zaporizhzhya, Ukraine

² Taurian State Agrotechnology University, 18, B. Khmelnitsky prosp., 72310 Melitopol, Ukraine

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In the work, the approach to accounting low-amplitude irregularities of the nanofilm surface has been proposed in the free-electron model and the finite depth potential well model. The electron energy spectrum and the size oscillations of the Fermi energy of metal films with a rough surface have been calculated within the boundary shape perturbation method. The relationship between the nature of the surface relief, amplitude of irregularities, material parameters and the behavior of the relative Fermi energy has been established. The calculations have been carried out for Al, Cu, and Au nanofilms.

Keywords: Fermi energy, Metal nanofilm, Roughness, Oscillations, The boundary shape perturbation.

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1. INTRODUCTION

Metal 2D systems are the subject of intense theoretical and experimental studies in recent years due to the improvement of technologies for producing continuous nanometer layers [1-7]. In these structures, the energy characteristics (Fermi energy, work function, surface energy) depend on the film thickness and have an oscillating behavior.

In the vast majority of cases, the study of metal 2D structures is based on the assumption of homogeneity of nanofilms in thickness. However, in practice, production of perfectly smooth layers is impossible. The thickness variations occur due to the granular structure of a real film and have sizes from a few tenths of a nanometer and more. The electron mean free path is the same in magnitude. Moreover, it is shown in the experimental work [8] that the presence of a rough surface leads to a nonmonotonic behavior of the differential voltage-current characteristics near the Fermi energy and to changes in tunneling conductance. The importance of taking into account the features of the size dependence of the Fermi energy is also caused by the fact that it gives the main contribution to the optical absorption [9].

Thus, the theoretical calculations, which describe the phenomena associated with the size quantization effects, require correction.

To take into consideration the nanofilm inhomogeneity in thickness, the choice of approach depends on the type of inhomogeneity. The adiabatic approximation and the Namba model are used for smooth inhomogeneities [10]. However, these methods cannot be applied to films with a stochastic surface relief. The method based on the transition in the Schrödinger equation to a new coordinate system, in which the film surface is smooth, is most often used for such systems [11]. The advantage of this approach is the ability to isolate the perturbation caused by the film inhomogeneity in thickness, in explicit form, not be limited to adiabatic approximation; but the obtained Hamiltonian is not Hermitian.

To describe a rough surface, the authors of [12, 13] have used the fractal approach, the peculiarity of which is that the fractal surface assumes self-similarity on all

scales. However, physical objects, in particular, nanofilms, due to the presence of the minimal characteristic scale, are not mathematically fractal. Therefore, as shown in [8], the use of the fractal description of a rough surface leads to non-physical results. Moreover, the authors of [8, 14] consider an approach where a random film boundary is described by a Gaussian function. However, the use of this approach greatly complicates the calculations of the energy spectrum and the density of states. Therefore, in this paper, for the calculation of the spectrum, we propose the use of a simpler "boundary shape variation" method, known in nuclear physics, continuum mechanics and physics of low-dimensional systems (see [15, 16] and references therein). The advantage of this approach is that the random inhomogeneity of the nanofilm surface in the first order of the perturbation theory can be taken into account by modifying the boundary conditions for the zero-approximation wave function, since the correction to the Hamiltonian (by analogy with [16]) is proportional to the square of the relative amplitude of the inhomogeneity, and, thus, it cannot be taken into account.

The aim of this work is to investigate the influence of surface roughness of nanometer metal films on the Fermi energy oscillations in the boundary shape perturbation method.

2. STATEMENT OF THE PROBLEM AND BASIC RELATIONS

We suppose that the conduction electrons of a thin metal film of thickness L are in a rectangular potential box of depth $U_0 < 0$, whose shape repeats the shape of a film with smooth surfaces. The longitudinal film sizes are much larger than the film thickness ($a, b \gg L$). In this case, quantization of the transverse component of the momentum manifests itself that leads to the formation of subbands.

Unperturbed states in the film are described by the following wave functions:

$$\Psi(x, y, z) = \frac{1}{\sqrt{ab}} \psi_m(x) e^{\frac{2\pi n y i}{a}} e^{\frac{2\pi p z i}{b}}, \quad (1)$$

* andko@zntu.edu.ua

where $n = \pm 1, \pm 2, \dots$; $p = \pm 1, \pm 2, \dots$; $m = \pm 1, \pm 2, \dots$; and $\psi(x)$ is equal to

$$\psi_m(x) = \begin{cases} B_1 e^{i_m x}, & x < -\frac{L}{2}; \\ A_1 \cos k_{xm} x + A_2 \sin k_{xm} x, & -\frac{L}{2} < x < \frac{L}{2}; \\ B_4 e^{-i_m x}, & x > \frac{L}{2}. \end{cases} \quad (2)$$

Here $i_m = \sqrt{k_0^2 - k_{xm}^2}$; $\hbar^2 k_0^2 = 2m_e U_0$; m_e is the electron mass.

Considering the film is rough and the inhomogeneity is small ($\xi = h/L \ll 1$, where h the maximum roughness amplitude), one can use the boundary shape perturbation method. Expanding the wave function $\psi(x)$ and its derivative on the boundaries $x = \pm L/2$ into a Taylor series, it is possible to write

$$(i_m^2 - k_{xm}^2) \sin k_{xm} L + 2i_m k_{xm} \cos k_{xm} L = \xi k_{xm} L \left(k_{xm}^2 \cos k_{xm} L - i_m^2 \cos^2 \frac{k_{xm} L}{2} + \frac{3}{2} i_m k_{xm} \sin k_{xm} L \right). \quad (4)$$

The size dependence of the Fermi energy is determined by the solution of the transcendental equation [17]

$$m_F \varepsilon_F = \frac{\pi \hbar^2}{m_e} L \bar{n} + \sum_{m=1}^{m_F} \varepsilon_m; \quad \varepsilon_i \leq \varepsilon_F; \quad m = 1, 2, \dots, m_F, \quad (5)$$

where ε_m is the energy of the m -th electron subband, to which the wave function $\psi_m(x)$ corresponds; m_F is the number of the last occupied or partially occupied subband; \bar{n} is the conduction electron concentration in 3D metal.

3. RESULTS AND DISCUSSION

The calculations were performed for Al, Cu, and Au nanofilms with convex ($h > 0$) and concave ($h < 0$) relief, electron concentration $\bar{n} = 3/4\pi r_s^3$ with the average distance between electrons $r_s = 2.07a_0$, $2.11a_0$, and $3.01a_0$, respectively (a_0 is the Bohr radius).

The calculation results of the size dependences of the Fermi energy for the Cu film are illustrated in Fig. 1.

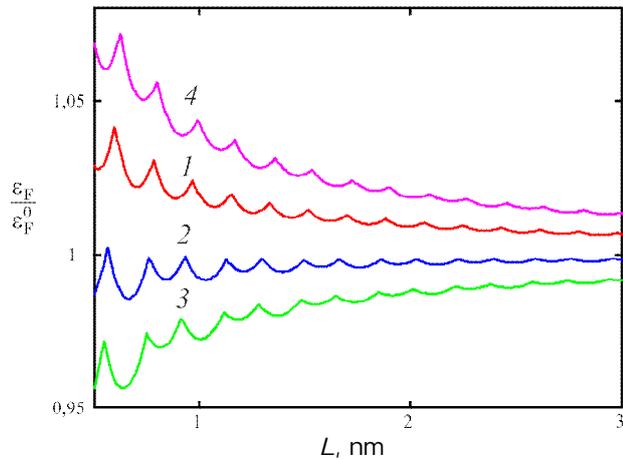


Fig. 1 – Size dependence of the Fermi energy of the Cu films for different values of the inhomogeneity amplitude: 1 – $h = 0$; 2 – $h = 0.05$ nm; 3 – $h = 0.1$ nm; 4 – $h = -0.05$ nm

$$\begin{aligned} \psi_1 \left(-\frac{L}{2} \right) - \xi \frac{L}{2} \frac{d\psi_1}{dx} \Big|_{x=-\frac{L}{2}} &= \psi_2 \left(-\frac{L}{2} \right) - \xi \frac{L}{2} \frac{d\psi_2}{dx} \Big|_{x=-\frac{L}{2}}; \\ \psi_2 \left(\frac{L}{2} \right) + \xi \frac{L}{2} \frac{d\psi_2}{dx} \Big|_{x=\frac{L}{2}} &= \psi_3 \left(\frac{L}{2} \right) + \xi \frac{L}{2} \frac{d\psi_3}{dx} \Big|_{x=\frac{L}{2}}; \\ \frac{d\psi_1}{dx} \Big|_{x=-\frac{L}{2}} - \xi \frac{L}{2} \frac{d^2\psi_1}{dx^2} \Big|_{x=-\frac{L}{2}} &= \frac{d\psi_2}{dx} \Big|_{x=-\frac{L}{2}} - \xi \frac{L}{2} \frac{d^2\psi_2}{dx^2} \Big|_{x=-\frac{L}{2}}; \\ \frac{d\psi_2}{dx} \Big|_{x=\frac{L}{2}} + \xi \frac{L}{2} \frac{d^2\psi_2}{dx^2} \Big|_{x=\frac{L}{2}} &= \frac{d\psi_3}{dx} \Big|_{x=\frac{L}{2}} + \xi \frac{L}{2} \frac{d^2\psi_3}{dx^2} \Big|_{x=\frac{L}{2}}. \end{aligned} \quad (3)$$

After substitution of (2) into (3) and subsequent simplification, we obtain in the linear in ξ approximation (see Appendix A) the following equation for determining the energy spectrum:

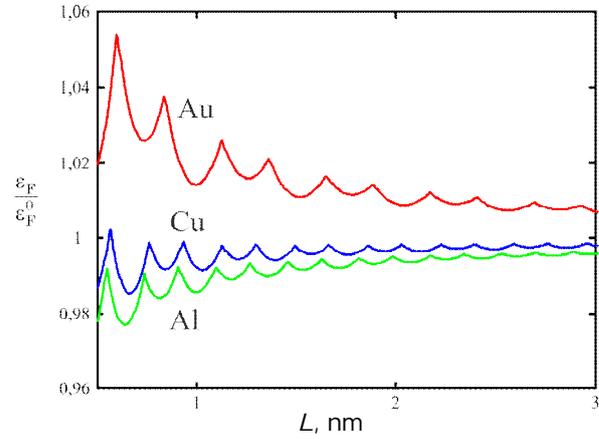


Fig. 2 – Size dependence of the Fermi energy for the films of different metals at $h = 0.05$ nm

As seen from the figure, the qualitative behavior of the size dependence remains. Thus, the maxima are achieved in all cases for the same values of L , and with increasing L the oscillation amplitudes decrease. Quantitatively, the values of $\varepsilon_F / \varepsilon_F^0$ for the case of rough films are 2-4 % lower compared with a perfectly smooth film. It also turns out that for the Cu films, $\varepsilon_F / \varepsilon_F^0 < 1$ at $h = 0.05, 0.1$ nm.

Fig. 2 shows the size dependences of the Fermi energy of different metals at the fixed value of the inhomogeneity amplitude $h = 0.05$ nm. As seen from Fig. 2, for Al and Cu films, the greater the magnitude of the inhomogeneity is, the smaller the Fermi energy is. The quantitative difference in the results for these cases is that the oscillation amplitudes in the case of Au are much larger than those for the case of Cu and Al. This is due to the fact that the oscillation amplitude is determined by the value of π / k_F^0 , which is the least for Al. A decrease in the Fermi energy of rough films of various metals with convex relief is explained by an increase in the “average” width of the potential well and, correspondingly, by the depression of energy levels.

4. CONCLUSIONS

The influence of surface roughness of metal 2D systems on the size oscillations of the Fermi energy has been studied in this work. In the framework of the boundary shape perturbation method, the electron energy spectrum in rough films of a nanometer thickness has been calculated. A comparison with the case of a film with a perfectly smooth surface has been performed.

It is established that regardless of the nanofilm material, the Fermi energy decreases with increasing inhomogeneity amplitude. This is associated with an increase in the "average" width of the potential well and the depression of energy levels. In the case of concave surface relief, a reverse effect is observed: an increase in the relative Fermi energy.

It is shown that for Cu films with convex surface relief, the Fermi energy values are lower than for the case of a bulk metal.

Moreover, the Fermi energy oscillation amplitudes for Al films are much higher than those for Cu films that is explained by a higher value of ϵ_F^0 for the case of Al.

APPENDIX A DERIVATION OF THE EQUATION FOR DETERMINING ENERGY SPECTRUM

We present a procedure for obtaining equation (4). Substituting the values of the functions and their derivatives in the points $x = \pm L/2$ into the boundary conditions (3), we derive the following homogeneous system of linear algebraic equations:

$$\begin{cases} B_1 e^{-i m \frac{L}{2}} - B_1 \xi \frac{L}{2} i m e^{-i m \frac{L}{2}} = A_1 \cos \frac{k_{xm} L}{2} - A_2 \sin \frac{k_{xm} L}{2} - \xi \frac{L}{2} k_{xm} \left(A_1 \sin \frac{k_{xm} L}{2} + A_2 \cos \frac{k_{xm} L}{2} \right); \\ B_4 e^{-i m \frac{L}{2}} - B_4 \xi \frac{L}{2} i m e^{-i m \frac{L}{2}} = A_1 \cos \frac{k_{xm} L}{2} + A_2 \sin \frac{k_{xm} L}{2} + \xi \frac{L}{2} k_{xm} \left(-A_1 \sin \frac{k_{xm} L}{2} + A_2 \cos \frac{k_{xm} L}{2} \right); \\ i m \left(B_1 e^{-i m \frac{L}{2}} - B_1 \xi \frac{L}{2} i m e^{-i m \frac{L}{2}} \right) = k_{xm} \left[A_1 \sin \frac{k_{xm} L}{2} + A_2 \cos \frac{k_{xm} L}{2} + \xi \frac{L}{2} k_{xm} \left(A_1 \cos \frac{k_{xm} L}{2} - A_2 \sin \frac{k_{xm} L}{2} \right) \right]; \\ i m \left(B_4 e^{-i m \frac{L}{2}} - B_4 \xi \frac{L}{2} i m e^{-i m \frac{L}{2}} \right) = k_{xm} \left[A_1 \sin \frac{k_{xm} L}{2} - A_2 \cos \frac{k_{xm} L}{2} + \xi \frac{L}{2} k_{xm} \left(A_1 \cos \frac{k_{xm} L}{2} + A_2 \sin \frac{k_{xm} L}{2} \right) \right]. \end{cases} \quad (\text{A.1})$$

The system (A.1) will have a solution under the condition that its determinant is equal to zero. Therefore,

we can write

$$\begin{aligned} & i_m^2 \left(\sin k_{xm} L + \xi L \cos^2 \frac{k_{xm} L}{2} \right) - k_{xm}^2 \left(\sin k_{xm} L + \xi L k_{xm} \cos k_{xm} L - \xi^2 \frac{L^2}{4} k_{xm}^2 \sin k_{xm} L \right) + \\ & + i_m k_{xm} \left(2 \cos k_{xm} L - \frac{3}{2} \xi L k_{xm} \sin k_{xm} L + \xi^2 \frac{L^2}{4} k_{xm}^2 (1 - \cos k_{xm} L) \right) = 0. \end{aligned} \quad (\text{A.2})$$

After dropping the terms proportional to ξ^2 in the ex-

pression (A.2), we come to the equation (4).

REFERENCES

- Pucci, F., Kost, G., Fahsold, M., Jalochowski, *Phys. Rev. B* **74**, 125428 (2006).
- M. Hövel, B. Gompf, M. Dressel, *Phys. Rev. B* **81**, 035402 (2010).
- S. Laref, J. Cao, A. Asaduzzaman, K. Runge, P. Deymier, R.W. Ziolkowski, M. Miyawaki, K. Muralidharan, *Opt. Expr.* **21**, 11827 (2013).
- W. Ming, S. Blair, F. Liu, *J. Phys.: Condens. Matter.* **26**, 505302 (2014).
- M. Lončarić, J. Sancho-Parramon, H. Zorc, S. Šegota, P. Dubček, S. Bernstorff, *Thin Sol. Films* **591**, 204 (2015).
- A.V. Korotun, Ya.V. Karandas, *J. Nano-Electron. Phys.* **7** No 2, 02018 (2015).
- S.W. Kim, L. Pang, B. Hong, J. Ptasinski, Ye. Fainman, *Opt. Lett.* **41**, 1522 (2016).
- V.D. Borman, P.V. Borysyuk, O.S. Vasylyev, M.A. Pushkyn, V.N. Tronyn, Y.V. Tronyn, V.Y. Troyan, N.V. Skorodumova, B. Yohansson, *ZhETF Lett.* **86**, No 6, 450 (2007).
- V.P. Kurbatskiy, A.V. Korotun, V.V. Pohosov, *Ukr. J. Phys.* **53**, 569 (2008).
- R.I. Bihun, Z.V. Stasyuk, O.A. Balitskii, *Phys. B* **487**, 73 (2016).
- Z. Teanović, M.V. Jarić, S. Maekawa, *Phys. Rev. Lett.* **57**, 2760 (1986).
- A.A. Potapov, *Fraktaly v radiofizike i radiolokatsii: Topologiya vyboriki* (Moskva: Universit. kniga: 2005).
- R.C. Munoz, C.A. Gonzalez-Fuentes, R. Henriquez, A. Espinosa, G. Kremer, L. Moraga, A. Ibañez-Landeta, S. Bahamondes, S. Donoso, M. Flores, *J. Appl. Phys.* **110**, 023710 (2011).
- S. Chatterjee, A.E. Meyerovich, *Phys. Rev. B* **84**, 165432 (2011).
- V.P. Dzyuba, Yu.N. Kul'chin, V.A. Milichko, *Phys. Solid State* **56**, 355 (2014).
- A.V. Korotun, *Phys. Solid State* **56**, 1197 (2014).
- V.P. Kurbatskiy, V.V. Pogoso, *Phys. Solid. State* **46**, 526 (2004).