Effect of Geometry on the Fermi Energy Of Metallic Nanowire

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The metal wires on semiconductor or dielectric substrates can be considered as one-dimensional electron systems with properties, which are of interest both from the fundamental point of view and from the perspective of their application in nanoscale electronic devices. As a rule, the calculation of the energy spectrum performed for the specific geometry of the metal sample and to obtain the approximate solutions of the Schrödinger equation. The Fermi energy size behavior, in particular, makes a major contribution to the optical conductivity [1, 2]. The solutions for metallic wires with circle cross section are known. However, in experimental conditions the simple geometry delays due to transverse stress or lateral pressure and is close to elliptical one. Therefore, the problem of the Fermi energy calculation for the elliptical nanowires is important.

It is assumed that the conduction electrons of the wire are located in a rectangular potential box with hard walls, so that the box shape reproduces the wire with elliptical cross section. There are exact solutions of the Schrödinger equation [3]. We start from the expression for the energy of an electron $\varepsilon_{mnp} = \hbar^2(k_{mn}^2 - k_{zp}^2)/2m$, where k_{mn}^2 and k_{zp}^2 are the eigenvalues of transverse and longitudinal components of the electron wave vector, respectively. From equality of the total number of the occupied states to the number of the conduction electrons $\overline{n}$ we obtain the equation for the computation of the Fermi level

$$\overline{n} = \frac{2}{\pi^2 ab}\sum_{m,n}\sqrt{k_{\mathrm{F}}^2 - k_{mn}^2},$$

where a and b are the half-axes of the ellipse. The summation should be performed over all numbers $m = 0,\pm1,\pm2,\ldots$ and $n = 0,1,2\ldots$ satisfying the condition $k_{mn} \le k_{\mathrm{F}}$. The calculations performed for wide range of sizes a and b and compared with the results for wires with equivalent cross sections.

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