Semi-infinite jellium: thermodynamic characteristics

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Currently, the most common method for the study of metals, including the interface, is density functional theory (DFT) [1]. But in essence it is quantum-mechanical method and therefore it does not allow to calculate the thermodynamic properties of metal. An alternative to DFT is proposed in papers [2,3] quantum-statistical theory of semi-bounded metal, which allows to calculate structural and thermodynamic properties with correct account of many-body effects.

We present a study of the grand thermodynamic potential $\Omega(T, V, \mu)$ (T is temperature, V is volume, μ is chemical potential) of semi-infinite jellium. For the calculation of this potential the method of functional integration [2,3] is used.

Proceeding from the

$$N = -\left(\frac{\partial\Omega(T, V, \mu)}{\partial\mu}\right)_{T,V}$$

(N is the number of electrons) nonlinear algebraic equation for the chemical potential μ electron subsystem of semi-infinite jellium is obtained. This equation for the chemical potential μ in the case of low temperatures ($\beta\mu \gg 1$) for different models of the surface potential [1,2] is solved numerically. Also the numerical calculation of entropy and pressure for semi-infinite jellium is done.

[1] Dreizler R. M., Gross E. K. U. Density functional theory. Springer, 1990, 317 p.
[2] Kostrobij P. P., Markovych B. M. Condens. Matter Phys. 2003. **6**, 347.
[3] Kostrobij P. P., Markovych B. M. Condens. Matter Phys. 2008, **11**, 641.