LOW TEMPERATURE THERMODYNAMIC ADVANTAGE OF BI-INTERCALATE

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As today, the prospects of application of intercalated layered crystals as sources of power have been proven [1]. The increased interest in intercalated structures is also due to the possibility of high conductivity of intercalate (electronic or ionic) and its controllability. Moreover, the greater the amount of intercalate, the greater the capacity of power sources. Therefore, in order to increase the capacity the method of bi-intercalation [1], which greatly increases the Gibbs potential, is applied.

The thermodynamic potential of Gibbs, in the "guest-host" systems consists of a configuration of entropy and enthalpy components, which includes the interaction between guest components and change in the position of the Fermi level of electrons or holes as well as  − change of the lattice parameter etc. The entropy component prevails over the enthalpy one for small and large values of *х* (**). In the region of intermediate values, the enthalpy component may be decisive. There are a number of materials (*LiMn3O4*), where the electronic contribution determines the profile of the discharge curve. The lower the temperature, the more important becomes the electronic input into the enthalpy component. Therefore, trends in behavior of  depending on the microscopic parameters, in particular the features of the energy structure of the crystalline matrix, are key factors for understanding of the energy advantage of the bi-intercalation process.

For *Т=0* the free energy of the electronic subsystem coincides with the internal one *F* = *E*, and its change Δ*F* (Δ*F* = *F*2 – *F*1), calculated on the density of states found in [2] can serve as a test of thermodynamic utility or malfunction of the intercalated system. The dependence of free energy of the electronic subsystem of bi-intercalate is considered on the following parameters: 1) Fermi energy *εF*; 2) the concentration of free carriers *n*, taking into account the energy states of the intercalate *ε1, ε2;* 3) different concentrations of an intercalate *р*1 and *р*2, as well as the degree of layering of the crystal. The results of the calculations are compared with the similar [3], carried out for a layered crystal with one type of intercalate.

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2. Demkiv L.S. et.al. 2018 IEEE 8th International Conf. on nanomaterials Application&Properties, Zatoka, Ukraine, September 9-14, 2018.
3. Tovstyuk N.K. Low Temperature Physics – 2004. – V.30, №6. – P. 672 – 678.