THERMODYNAMICS OF LITHIUM INTERCALATION INTO GRAPHITE NANOFLAKES

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Carbon nanostructures are widely used as electrode materials for energy storage and accumulation devices. Graphene, a single layer of sp^2-hybridized carbon atoms, is one of the most promising carbon allotropes. Various approaches have been developed to improve the performance of graphene-based materials. In particular, the introduction of heteroatoms into their composition alters their electrochemical properties [2]. In the present study, N-, P-doped graphene nanoflakes (GNFs) were obtained.

Electrode charge-discharge processes, involving the transformation of chemical compounds into others, entail changes in thermodynamic functions: the free Gibbs energy ΔG, entropy ΔS, and enthalpy ΔH. Knowledge of these parameters allows for the prediction of electrochemical processes occurring in the system [3]. However, the thermodynamics of lithium intercalation into the GNFs structure have not been addressed in the literature.

In this study, we analyzed the thermodynamic functions of lithium intercalation into the -N, -P structures of GNF in a 1 M $LiPF_6$ solution in a 1:1 mixture of ethylene carbonate and diethylene carbonate, EC + DEC. The measurements were carried out in coin-cells using galvanostatic intermittent titration technique and OCV measurements in the temperature range of 20-50°C. The parameters were evaluated using known equations [3]:

$$\Delta G = -nFE_{OCV},$$
$$\Delta S = -nF\frac{\partial E_{OCV}}{\partial T}.$$

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This work was supported by the Russian Science Foundation, grant № 25-23-00117.