THEORETICAL STUDY OF STRUCTURAL TRANSFORMATIONS AT FULLERIT HYDROGENATION. HYDROGEN SOLUBILITY

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The investigation of processes of fullerenes hydrogenation and dehydrogenation is of interest to scientists and engineers in connection with their different practical applications which includes also the elaboration of the systems of hydrogen accumulation and storage.

Theoretical study of structural phase transition from simple cubic lattice (SCL) to body-centered (BCCL) in fullerit at its hydrogenation has been conducted. On the basis of molecular-kinetic concept the calculation of crystal free energy has been carried out taking into consideration the interaction of nearest fullerenes $\Phi_1\Phi_1$, $\Phi_2\Phi_2$, $\Phi_1\Phi_2$ ($\Phi_1=C_{60}$, $\Phi_2=C_{70}$), as well as fullerenes interaction with hydrogen atoms Φ_1H, Φ_2H and also interaction between hydrogen atoms HH. The dependence of free energy on temperature, fullerit composition, hydrogen concentration, its activity and energetic parameters has been derived. The temperature of transition between phases of SCL⇔BCCL type at fullerit hydrogenation has been calculated, the conditions of its implementation have been determined. The phase diagrams defined the temperature of SCL⇔BCCL transformation as a function of hydrogen content has been constructed. The temperature dependence of hydrogen solubility in fullerit has been calculated. The increase and decrease conditions of hydrogen solubility with temperature rise have been ascertained. The results of theoretical calculations have been compared with experimental data. These calculations permits to explain and substantiate the structural transitions of fullerit at its hydrogenation, to show that these changes are the result of elevated temperature and also to give grounds of possibility of fullerenes hydrides formation in their simplest form at the solid-phase hydrogenation.

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