Atomic mechanisms and characteristics of diffusion, sorption and intercalation of hydrogen in nanographite and graphene structures

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On the basis of results [1-10] of thermodynamic analysis of a number of the most cited experimental and theoretical data, the atomic mechanisms and characteristics of diffusion (Eqns. 1, 2), sorption (including some chemisorption (Fig. 1)) and intercalation of hydrogen in nanographite and graphene structures are considered.

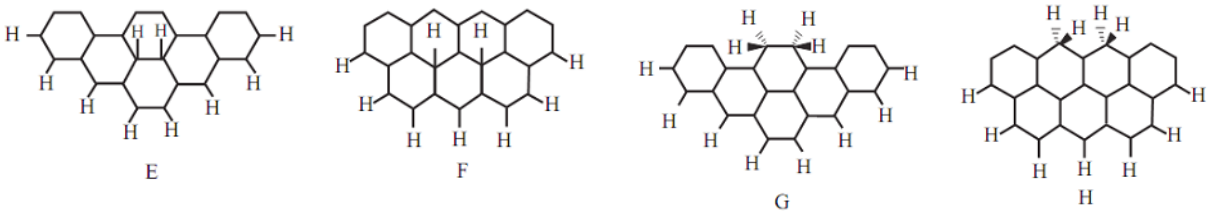

Fig. 23: Some theoretical models of chemisorption of atomic hydrogen on the basal and edge planes of graphite: "F" – process III (ΔH_{III} = -2.5 eV); "H" – process IV (ΔH_{IV} = -3.7 eV).

According [1-4], the apparent diffusion coefficient ($D_{III,IV}$) and the apparent activation energy ($Q_{III,IV}$) of diffusion of hydrogen atoms in nanographite and graphene structures are described as:

$$D_{III,IV} \sim (D / K_{III,IV}) \, , \, Q_{III,IV} = (Q - \Delta H_{III,IV}) \approx -\Delta H_{III,IV}, \qquad (1, 2)$$

where D and Q ($\approx$ 0.1 eV) are the quantities for the case without the chemisorption ifluence, $K_{III,IV}$ are the related equilibrium constants, $\Delta H_{III,IV}$ are the chemisorption energies.

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