Kubas interaction of hydrogen molecules with a lithium silicate glass network

Efimchenko V ${\bf S}^{1,@},$ Korotkova M ${\bf A}^1,$ Meletov K ${\bf P}^1$ and Buchner ${\bf S}^2$

¹ Institute of Solid State Physics of the Russian Academy of Sciences,

Akademika Osipyana Street 2, Chernogolovka, Moscow Region 142432, Russia ² Universidade Federal do Rio Grande do Sul, Rua/Streat: Teixeira de Freitas 538, Ap. 301. , Porto Alegre 90640-22, Brazil

[@] efimchen@issp.ac.ru

The effect of lithium cations on the interaction of molecular hydrogen with the silicate network was studied by measuring the thermal stability of concentrated solid solutions of molecular hydrogen $Li_2O \bullet 6SiO_2 - 0.39H_2$ and $Li_2O \bullet 6SiO_2 - 0.25H_2$ synthesized at high pressures. According to the Raman data, the hydrogenated $Li_2O \bullet 6SiO_2$ glass contained hydrogen in the molecular form. The kinetics of decomposition of the solutions was studied by Raman spectroscopy and by hot hydrogen extraction during isothermal annealing in a pre-evacuated volume at T = 273 - 370 K. Raman spectroscopy showed that the decomposition reactions of these solutions had close activation energies of $E_a = 427$ and 486 meV, respectively. The activation energies determined by the hot extraction were $E_a = 185$ and 192 meV, or more than twice as small. At the same time, all these values exceeded the characteristic energy for the Van-der-Waals forces, which suggests a strong Kubas interaction between the H₂ molecules and lithium silicate network. The work was supported by the Russian Science Foundation, project No. 23-23-00426.