

Temperature dependent adsorption behavior of hydrogen molecules in Multi-walled Carbon Nanotubes

Zheng Qing-Rong * Gu An-Zhong Lu Xue-Sheng Lin Wen-Sheng

(Institute of Refrigeration and Cryogenics, Shanghai Jiaotong University, Shanghai 200030, P.R.C)

Abstract

The physical properties and behaviors of hydrogen molecules within the micro-pores of carbon adsorbents have not been clearly understood. However, they are key factors in interpretation of Hydrogen-Carbon interaction mechanism, which is relevant to the prospect of carbon adsorbents as hydrogen storage mediums.

In this paper, hydrogen adsorption data volumetrically measured on the Multi-walled Carbon Nanotubes (MWCNTs) sample in a wide range of temperature and pressure are applied to study the adsorptive mechanism. For the location of the temperature that can make full use of the physical adsorption performance without inhibiting the chemical adsorption of hydrogen molecules, a thermodynamic equilibrium based adsorption equation, which considers the interaction energy of the adsorbed hydrogen molecules and the adsorption potential, is developed to ascertain the relationship between temperature and the repulsion energy among the adsorbed hydrogen molecules at each equilibrium state.

From the analyzed results, it shows that the interaction energies among the adsorbed hydrogen molecules are positive in low temperature region (<200 K) and reach the highest value in the temperature range 160 ~180 K, but will be negative when the temperature is above 230 K. That is, the repulsion among the adsorbed hydrogen molecules is prominent in low temperature. However, the attraction in higher temperature is hard to be interpreted because the pressures are also high in those cases. Conclusions are drawn that the forming of C-H bond in MWCNTs should be considered at higher temperatures, and the temperature range 160~180 K will be both beneficial to the physical and chemical adsorption of hydrogen molecules in MWCNTs.