Quasielastic Neutron Scattering of Hydrogen Adsorbed in KC$_{24}$

JUSTIN PUREWAL, JAMES KEITH, CHANNING AHN, BRENT FULTZ, California Institute of Technology, CRAIG BROWN, NIST Center for Neutron Research — Quasielastic neutron scattering (QENS) and volumetric techniques were used to study the adsorption of H$_2$ by the stage-2 potassium graphite intercalation compound KC$_{24}$. A zero-coverage sorption enthalpy of 8.5 kJ/mol was measured from H$_2$ isotherms recorded at 77 K and 87 K. The saturation H$_2$ adsorption amount at 77 K was 1.2 mass%, corresponding to a stoichiometry of KC$_{24}$(H$_2$)$_{2.0}$. Quasielastic neutron scattering spectra for KC$_{24}$(H$_2$)$_{1.0}$ were collected at temperatures between 40 K and 80 K on a chopper spectrometer and a backscattering spectrometer. Two distinct H$_2$ diffusion processes were identified with characteristic times of approximately $\tau = 10$ ps and $\tau = 350$ ps at 60 K, respectively. By operating the backscattering spectrometer in fixed window mode, the total elastic scattering of KC$_{24}$(H$_2$)$_{1.0}$ was measured as a function of temperature. A sharp decrease in elastic intensity was observed at 35 K due to the onset of quasielastic scattering. This was interpreted as a melting transition of the H$_2$ adsorbate in KC$_{24}$.

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