High Intensity Total Scattering for Hydrogen in Materials

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A neutron total diffractometer, NOVA, was constructed at J-PARC to analyze crystalline and non-crystalline structure of hydrogen storage materials. With the world's most intense pulsed neutron source of J-PARC, NOVA realizes short-time measurement of total scattering and low-resolution inelastic measurement. As a total diffractometer, NOVA covers a wide momentum transfer range, 0.01 $Å^{-1} \leq Q \leq 100$ $Å^{-1}$ ($Q = 2\pi/d$, where d is a lattice constant) with $\Delta Q/Q \sim 0.35\%$. It is feasible to measure the static structure factor $S(Q)$ with the order of several ten mg. If the sample amount is enough (~ several 100 mg), atomic pair distribution function which derived by the Fourier transformation of $S(Q)$ is reliable up to 200 Å. One of the main objects of NOVA is hydrogen storage mechanism in materials and H_2/D_2 gas atmosphere (up to 10 MPa, temperature range can be control from 50 K to 473 K) has been equipped on NOVA for *in-situ* observation of hydrogen absorption and desorption process. Another unique feature of NOVA is a capability of inelastic measurement to study vibrational state of hydrogen, which closely relates to bonding to surrounding atoms.

Some of recent results of structural analysis on NOVA will be presented.