MS44-P2 Analysis of short range phenomena in novel materials using the PDF-method

Philipp Hans[1], Reinhard B. Neder[2], Nastaran Hayati-Roodbari[3], Paul Kautny[4], Klaudia Hradil[1]

1. X-ray Centre, Vienna University of Technology
2. Crystallography and Structural Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg
3. Materials Science and Physics, University of Salzburg
4. Institute of Applied Synthetic Chemistry, Vienna University of Technology

email: philipp.hans@tuwien.ac.at

In the present contribution we will show results of pairdistribution function (PDF) studies on amorphous materials. The pair distribution function contains information on the occurrence of all atom-to-atom distances in the substance.

The samples consist of so called host materials for organic-light-emitting-diodes (OLEDs) and are applied as amorphous films. In this amorphous state their electronic structure seemingly gets altered in a way required to induce the light emittance in the blue region. The molecular structure of the molecules is known and these molecules posses a large degree of freedom with respect to internal torsion. The initial expectation was that the light emitting state is caused by collective torsion of neighbouring molecules.

Initial PDF data were collected on an inhouse powder diffractometer with Mo-radiation. The experimental PDF does not show correlations beyond intramolecular distances. This indicates that the material is highly disordered and does not show correlated tilts between neighbouring molecules. Refinements with the DISCUS-Suite confirm the local torsion and the lack of correlations.

Keywords: amorphous organic materials, PDF-analysis, glass structure

MS44-P3 In-situ measurements of average and local structures in hydrogen gas environment at BL22XU in SPring-8

Akihiko Machida[1], Naoyuki Maejima[1], Tetsu Watanuki[1], Hyunjeong Kim[2], Kouji Sakaki[2], Yumiko Nakamura[2]

1. Synchrotron Radiation Research Center, National Institutes for Quantum and Radiological Science and Technology, Sayo, Hyogo 679-5148, Japan
2. Reserch Institute of Energy Frontier, National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8565, Japan

email: machida@spring8.or.jp

Hydrogen absorbing alloys are considered as potential hydrogen storage materials for several applications such as stationary energy storage system. The absorbed hydrogen atoms largely expand the metal lattice and induce a structural phase transition on the hydrogenation reaction. From a nanoscale structural point of view, a large number of crystallographic defects, such as dislocations, are formed during hydrogen absorption/desorption cycles and they influence the properties of hydrogen absorbing alloys. Therefore, thorough structural studies on the hydrogen absorbing state are essential for improving the material properties as well as for preparing novel alloys. However, those are challenging tasks because the hydrogen absorbing states of alloys usually arise in the pressurized hydrogen gas environment. Furthermore, average structural information from conventional methods is not sufficient to elucidate the mechanism of hydrogen absorption, and therefore local structural information is also necessary.

In order to investigate the structural change of hydrogen absorbing alloys during hydrogen absorption/desorption processes, we have developed in-situ setup for x-ray diffraction experiments at BL22XU in SPring-8. Using a large imaging plate (IP) detector and high energy x-rays about 70 keV, we can also obtain x-ray total scattering data (Q_{max} ~ 27 Å^{-1}) for the atomic pair distribution function (PDF) analysis, which is one of powerful methods to investigate structures in an atomic scale. PDFs obtained from BL22XU show peaks even above 100 Å allowing us to investigate even intermediate range structural features related to the crystallographic defects or crystal lattice distortion. Recently, we have developed time-resolved measurement setup using an amorphous-Si detector from PerkinElmer. This setup enables us to study change in both average and local structures of hydrogen absorbing alloys in either equilibrium or non-equilibrium states with hydrogen gas pressure up to 1 MPa. We succeed in obtaining the PDF of $La(Ni,Al)_5$ intermetallic compounds on hydrogen absorption process with short accumulation time of 0.25 sec. In this presentation, we will introduce our experimental setup and evaluation of obtained PDFs, and present some preliminary results on the hydrogen absorbing alloys.

This work is supported by Photon and Quantum Basic Research Coordinated Development Program from the Ministry of Education, Culture, Sports, Science and Technology, Japan.

Keywords: x-ray total scattering, in-situ measurement, hydrogen absorbing alloys