Contribution ID: **73** Type: **Oral Presentation**

Ultrasmall Angle Xray Scattering (USAXS) and WideAngle Xray Scattering (WAXS) Studies on the Complex Metal Hydride NaAlH4

This research seeks to understand the role of ScCl3, ZrCl4, and VCl3 catalysts in NaAlH4. Some researchers suggests that the catalyst serves to decrease the H2 gas desorption temperature in these materials by influencing the reaction rates. Others suggest that the catalyst acts more as a dopant, thereby mitigating (enhancing) diffusion rates is in the solid phases. Changes in the hydride powders during desorption occurs at multiple length scales. To study this problem, we have examined these hydrides at multiple length scales using an Xray scattering instrument which is capable of capturing nine decades of scattering intensity from a scattering wave vector, Q, of 0.0001Å to 6.0 Å . The ultrasmall angle Xray scattering (USAXS) instrument sector 9ID-D of the Advanced Photon Source (APS) offers the capability to simultaneously collect morphology information using USAXS and SAXS data while examining the crystallographic changes using wideangle
Xray scattering (WAXS) data. Studies were performed on aspurchased, neat, and catalyzed NaAlH during insitu heating up to 170C (just below the H desorption temperature for uncatalyzed NaAlH4). Results showed that NaAlH has a surface fractal (highly porous) morphology. Isothermal studies performed at 30C, 65C, 100C, 135C, and 170C reveals changes at low Q (Q˜.001 Å to 0.01 Å) associated with highly interconnected intraparticle porosity which is suitably described by a power-law slope for a Gaussian polymer chain structure of p˜2. At high scattering wave vector, Q˜0.03Å , the presence of a pore population which obeys Porod scattering and appears to have a size at 21nm is present. These fine pores increase in their population density as temperature is elevated. These morphological changes are all believed to occur because of hydrogen diffusion out of the powders. The WAXS data reveals thermal expansion to occur, but no solid state phase transformation to the product phase. Next steps will involve correlating these changes with hydrogen desorption temperatures for each catalyzed sample.

Authors: Prof. DOBBINS, Tabbetha (Rowan University); Dr ILAVSKY, Jan (Advanced Photon Source)

Presenter: Prof. DOBBINS, Tabbetha (Rowan University)

Session Classification: Material Physics

Track Classification: Material Physics