Atom Dynamic of Amorphous Materials $(Ni_{0.60}Nb_{0.4})_{100-x}Zr_x$ (x=0 to 30) by X-Ray Photon Correlation Spectroscopy, Neutron Studies

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Abstract:
The mitigation of greenhouse gas emissions on the environment led to the development of non-polluting hydrogen fuel cell use in automobiles. Syngas produced from coal gasification is converted to H_2 and CO_2 gasses by the water shift reaction [1-3]. Metallic membranes are used to separate H_2 from CO_2 and other gasses obtained from the water shift reaction of coal-derived syngas. Commercial crystalline Pd-Ag membranes are widely used for this purpose, however, Pd is an expensive strategic metal. Thus, inexpensive Ni-Nb-Zr amorphous alloys are studied. Amorphous membrane ribbons of $(Ni_{0.60}Nb_{0.40})_{100-x}Zr_x$ fabricated by melt-spinning method exhibit high permeabilities of hydrogen between 200-400ºC, however, the mechanism of permeation and the nature of the local atomic order of the amorphous membranes are not fully understood.

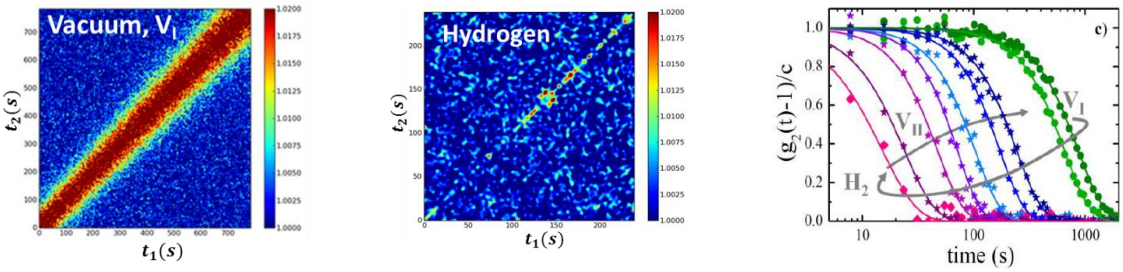

Figure 1. Reversible hydrogenation in binary $Ni_{60}Nb_{40}$ amorphous alloy: Two-time correlation function measured by XPCS at 373K (a) vacuum (b) hydrogenation (c) intensity correlation function in vacuum (V_I), hydrogenation (H_2) and finally dehydrogenation (V_{II})

In this study, atom dynamics of amorphous membranes is determined by synchrotron x-ray photon correlation spectroscopy (XPCS) with and without hydrogen at ESRF. This study revealed a dramatic reversible acceleration of the atomic motion under hydrogen atmosphere at low temperatures shown in the Figure 1. To understand high-pressure permeation behavior Raman Spectroscopy measurement and synchrotron x-ray diffraction are used with diamond anvil cells at CIW and APS. To understand hydrogen vibrational density of states, neutron vibrational spectroscopy (NVS) is performed at NIST center for neutron research. NVS result reveals hydrogen position inside Zr_4, Nb_4 destorted tetrahedral sides. Nearest neighbour distance (Ni-Nb/NiZr~ 0.268 nm, Nb-Nb~ 0.295 nm and Zr-Nb/Zr-Zr ~0.324 nm) and short range order (~1.8 nm) of these amorphous alloys are determined by Neutron Total scattering (HIPD). Atom probe tomography (APT) reveals Nb-rich (5-6 nm) and Zr-rich (~ 2 nm) clusters embedded in a Ni-rich matrix whose compositions deviates from the nominal overall composition of the membrane. Our DFT simulation reveals the icosahedra structure and cluster information which match with APT and HIPD results. Altogether, these studies show the atom dynamics with and without hydrogen, local atomic structure of the amorphous ribbon and cluster formation inside the membranes.
(This research is supported by US DOE-NNSA grant, DE-NA0002004 and DOE-NETL FE0000998).

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