

# Atom dynamics and Neutron Vibrational Spectroscopy NiNbZr Glassy Membranes

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Crystalline Pd/Pd-Ag membranes are generally used in hydrogen separation from CO<sub>2</sub> and other gases in power generation applications. Inexpensive amorphous Ni-based alloys are being developed as an alternative to expensive Pd alloys. Amorphous membrane ribbons of (Ni<sub>0.60</sub>Nb<sub>0.40</sub>)<sub>100-x</sub>Zr<sub>x</sub> fabricated by melt-spinning method exhibit high permeabilities of hydrogen between 200-400°C [1-4]. Atom probe tomography (APT) revealed Nb-rich and Zr-rich clusters embedded in a Ni-rich matrix whose compositions that deviated from the nominal overall composition of the membrane. Fukuhara et al. [5] reported icosahedral cluster arrangement of Ni-Nb-Zr atoms; we also found clusters based on APT and neutron SANS data, which can be interpreted as icosahedral arrangement. Neutron vibrational spectroscopy of these alloy yielded possible positions of hydrogen. Atom dynamic studies by X-ray photon correlation spectroscopy (XPCS) revealed a dramatic reversible acceleration of the atomic motion under hydrogen atmosphere at low temperatures; these effects are observed by standard thermodynamic/kinetic measurements. Dynamic mechanical analyses (DMA) indicated amorphous to amorphous phase transitions well below the recrystallization temperature, as well as the change elastic modulus as a function of temperature. Devitrification kinetics of these amorphous ribbons by using the John-Mehl-Avrami method showed Avrami exponents ranging from 1.92 to 2.47 indicating diffusion controlled 3-D growth mechanism. In an attempt to develop new alloys we show liquidus profiles for the ternary system using CALPHAD methodology. Hydrogen permeation, atom probe tomography, small angle neutron scattering, neutron vibrational spectroscopy, dynamic mechanical analyses, XPCS and devitrification kinetic aspects of these membranes will be presented.

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### **References:**

- 1. S. Sarker, D. Chandra et al, Applied Physics A, A 122, 168 (2016).
- 2. M.D. Dolan, N.C. Dave, A.Y. Ilyushechkin, L.D. Morpeth, K.G. McLennan, J. Membr. Sci. 285 (2006) 30
- 3. S.M Kim, D. Chandra et al, Journal of Non-Crystalline Solids, 358 (2012) 1165–1170.
- 4. S. Paglieri, N. Pal, D. Chandra, Journal of Membrane Science, 378 (2011) 42-50.
- 5. M. Fukuhara, N. H. Oji, A. Inoue, S. Emura, JALCOM, 497 (2010) 182–187

### Biography

Dhanesh Chandra is a Foundation Professor of Materials Science and Engineering in the College of Engineering at the University of Nevada, Reno. He has over 100 scientific publications, graduated 35 Ph.D and MS students. Member of Hydrogen IEA-Task 32, received over \$12 Million research funding, received Mackay School of Mines Dean's Outstanding Teaching award, received many Best Poster Awards from Denver X-Ray Conference over the years, sabbatical leaves at Los Alamos National Laboratory, University of Geneva, University of Paris (CNRS), Università di Roma "La Sapienza," and University of Freiburg. Organized 3 major International Energy Conversion Conferences, including a Special Hydrogen Research Symposium *"Advanced Materials for Energy Conversion III, In honor of Drs. G. Sandrock, L. Schlapbach, and S. Suda," Reviewed and co-edited* a proceeding by *D. Chandra*, et. al., 2006. Book chapter: D. Chandra, *"Intermetallics for Hydrogen Storage"* Edited by G. Walker, Woodhead Publishing (2008).