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Effects of Nano-confinement on Hydrogen Dynamics in TiCl3-Doped NaAlH4 Studied using Quasi-Elastic Neutron Scattering (QENS). TABBETHA DOBBINS, Dept. of Physics Astronomy, Rowan University, SHATHABISH NARASEGOWDA¹, Institute for Micromanufacturing, Louisiana Tech University, CRAIG BROWN², Dept. of Chemical and Biomolecular Engineering, University of Delaware, MADHUSUDANA TYAGI³, Center for Neutron Research, NIST, Gaithersburg MD, TIMOTHY JENKINS, Army Research Laboratory, Aberdeen Proving Ground, MD — Dynamics of hydrogen in 4 mol % TiCl3-doped NaAlH4 nanoconfined within the mesoporous SBA15 was studied using QENS. Results show a higher fraction of hydrogen is mobile within these nanoconfined systems relative to bulk TiCl3-doped NaAlH4 but with overall localized motion. Nanostructured Ti-doped NaAlH4 exhibited poorer long-range diffusion kinetics than bulk materials of the same composition. Around 15% of hydrogen participated in longrange motion at 400K (relative to 5% in bulk). Around 65% to 75% of all available hydrogen atoms are mobile at 400K in localized dynamics described by rotation of AlH_x units. Less than 10% hydrogen was mobile at higher temperatures of 420K and 450K, possibly because of the formation of Si-Al phases. Dynamic models indicate that nanostructured samples demonstrated slightly shorter jump lengths (2.09 Å to 2.16 Å) relative to bulk Ti-doped NaAlH4 (2.27 Å).

¹currently at Intel Corporation, Beaverton OR

²Center for Neutron Research, NIST, Gaithersburg MD

³Dept. of Materials Science and Engineering, University of Maryland, College Park, MD

Tabbetha Dobbins Dept. of Physics Astronomy, Rowan University

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