Hydrogen Storage in Cu-Li-Mg Alloys

M. HELENA BRAGA, GEORGE CHERTKOV, ALICE ACATRINEI, SAURABH KABRA, LUKE DAE-MEN, LANSCE-LC, LANL, Los Alamos, NM 87545, USA — CuMg has an orthorhombic crystal structure (Fddd) and does not form a hydride. However, CuLi$_{x}$Mg$_{2-x}$ (x ~ 0.11) has a hexagonal crystal structure (P6$_2$22), just like NiMg$_2$, a compound known for its hydrogen storage properties. A comparison between the phase diagrams of the systems Cu-Mg and Ni-Mg shows that these binary systems form compounds with similar stoichiometry. NiMg$_2$ is formed by peritectic reaction of the elements at 759 °C (1032 K) and CuMg$_2$ at 568 °C (841 K) by congruent melting. Since the energy of formation of the hydride is related to that of the primary alloy, it was hypothesized that CuLi$_{x}$Mg$_{2-x}$ might also be a hydrogen storage material similar to NiMg$_2$. Presumably, its advantage would be that it would release hydrogen at a lower temperature (possibly close to room temperature). In order to determine the properties of the hydrogenated (and deuterated) CuLi$_{x}$Mg$_{2-x}$ material, absorption/desorption experiments were performed at several temperatures and under different pressures of H$_2$ (and D$_2$). Neutron diffraction patterns and neutron vibrational spectra were collected to elucidate the behavior of hydrogen in the Li-doped CuMg$_2$ intermetallic.

1M.H. Braga acknowledges FCT for (SFRH/BSAB/791/2008) grant.
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Date submitted: 18 Nov 2008