

3.1.9 NEUTRON SCATTERING AND AB-INITIO SIMULATIONS TO CHARACTERIZE THE Cu-Li-Mg-H SYSTEM

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Keywords: Neutron Diffraction, Neutron Spectroscopy, Density Functional Theory (DFT), phonons, Cu-Li-Mg-H.

Our aim is to study the quaternary Cu-Li-Mg-H system. CuMg_2 has an orthorhombic crystal structure and does not form a hydride: it reacts reversibly with hydrogen to produce Cu_2Mg and MgH_2 . However, $\text{CuLi}_x\text{Mg}_{2-x}$ ($x = 0.08$) has a hexagonal crystal structure, just like NiMg_2 , a compound known for its hydrogen storage properties. NiMg_2 absorbs up to 3.6wt.% of H, at 1bar and 282°C. In spite of the fact that the percentage of hydrogen absorbed by NiMg_2 is enough to propitiate practical applications, the temperature at which the alloy desorbs hydrogen is much too high for practical applications. 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 at 759°C and CuMg_2 at 568°C. Since the energy of formation of the hydride is related to that of the primary alloy, it was hypothesized that $\text{CuLi}_x\text{Mg}_{2-x}$ 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. Preliminary studies at LANSCE showed that not only $\text{CuLi}_x\text{Mg}_{2-x}$ absorbs a considerable amount of hydrogen, but also releases it at a temperature in the range of 50-150°C. In order to determine the properties of the hydrogenated (and deuterated) $\text{CuLi}_x\text{Mg}_{2-x}$, absorption/desorption experiments were performed at several temperatures and under different pressures of H_2 (D_2). Neutron diffraction patterns and neutron vibrational spectra were collected to elucidate the behaviour of hydrogen in the Li-doped CuMg_2 intermetallic (see figure on next page). Using DFT and phonon calculations we were able to determine the best value for x in $\text{CuLi}_x\text{Mg}_{2-x}$ and obtain its Gibbs energy as a function of temperature.

