Neutron spectroscopy of gamma-MgH2

ALEXANDER KOLESNIKOV, Oak Ridge National Laboratory; VLADIMIR ANTONOV, VADIM EFIMCHENKO, Inst. Solid State Phys. RAS, Chernogolovka, Russia; GARRETT GRANROTH, Oak Ridge National Laboratory; S.N. KLYAMKIN, Moscow State Un., Russia; A.V. LEVCHENKO, MICHAEL SAKHAROV, Inst. Solid State Phys. RAS, Chernogolovka, Russia; YANG REN, Argonne National Laboratory; TIMMY RAMIREZ-CUESTA, ISIS, Rutherford Appleton Laboratory, UK — Under ambient conditions, magnesium dihydride exists in two forms, alpha-MgH2 (the most stable modification) and gamma-MgH2 (a less stable modification). The alpha-phase partly transforms to gamma-MgH2 in the course of ball-milling and under high pressure and temperature. Due to the high hydrogen content of 7.6 wt.%, MgH2 has been intensively studied as a prospective material for hydrogen storage. By exposing of alpha-MgH2 to a pressure of 5 GPa and temperature 840 K, we prepared a sample, in which about 60% of the alpha-MgH2 was transformed to gamma-MgH2. We have measured inelastic neutron scattering (INS) spectra of both the high pressure treated MgH2 and starting alpha-MgH2, and extracted the spectrum for gamma-MgH2. The differences between the INS spectra and their agreement with the first-principles calculations for these compounds will be discussed.