Magnetic Effect on the Crystal Structure of Alpha-MnH0.07

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Introduction

A recent high-pressure study showed that the solubility of hydrogen in alpha-Mn can be increased up to a few atomic percent [1]. The crystal structure of a powder sample of alpha-MnH0.07 synthesized under high hydrogen pressure was studied by neutron diffraction [2]. The cubic unit cell of the alpha-Mn structure, space group I-43m, contains 58 atoms positioned on the four crystallographically inequivalent sites 2a, 8c, 24g1, and 24g2.

The profile analysis of the neutron diffraction patterns of MnH0.07 showed that hydrogen randomly occupies interstitial positions 12e (0,0,0.538) inside distorted octahedra of manganese atoms on 24g1 and 24g2 sites. The 12e sites form “dumbbells” that are 0.68 Å long and positioned rather far apart, at the centers of the edges and faces of the unit cell of alpha-Mn with a = 8.9403 Å.

Methods and Materials

An extrapolation of the Mossbauer data [3] to the hydrogen content of the sample studied in this work shows that alpha-MnH0.07 should be antiferro-magnetically ordered below a Néel temperature of about 140 K. The Néel temperature of pure alpha-Mn is about 95K. The crystal structure of the alpha-Mn is tetragonal below its Néel point, with a crystal symmetry of I-42m. The tetragonal distortion, a/c, is very small, about 1.0003 [4].

Inelastic neutron scattering (INS) studies [2, 5] of alpha-MnH0.07 revealed a band of optical hydrogen vibrations split into three, in accordance with the low site symmetry of the hydrogen positions, and also a strong peak at 6.4 meV, which was attributed to the splitting of the vibrational ground state of hydrogen due to tunneling between the adjacent 12e sites. The results of INS studies that include the temperature and the neutron momentum transfer dependencies of the INS spectra of alpha-MnH0.07 at 5–200K (measured with the Time Focused Crystal Analyser [TFXA] at ISIS, MARI spectrometer at ISIS, and IN6 spectrometer at the Institut Laue-Langevin [ILL]) and the INS spectra of alpha-MnD0.05 at 1.7-180K (measured with the IN6 and IN1 BeF spectrometers at ILL) support the tunneling origin of the peak.

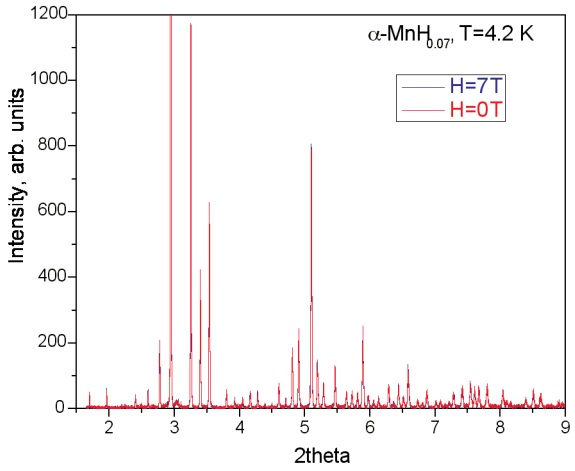

FIG. 1. X-ray diffraction pattern (lambda = 0.10775 Å) of alpha-MnH0.07 measured at a temperature of 4.2K with a magnetic field of H = 7 T and without a magnetic field.

Discussion

The remarkable features of the hydrogen tunneling peak in the INS spectrum of alpha-MnH0.07 are its anomalously large integral intensity compared to that of the optical hydrogen band and its anomalously high energy of 6.3 meV, which is about 30 times higher than the energy of tunneling splittings found for hydrogen in other metals [6]. Hydrogen tunneling in alpha-MnH0.07 is one of very few quantum effects observed at temperatures as high as 100K. Hydrogen tunneling in metals was earlier observed only at temperatures below 10K.

In the present experiments, we studied the effect of magnetic field on the crystal structure of alpha-MnH0.07. We carried out x-ray measurements at temperatures T of 4.2, 90, and 140K without a magnetic field and in a magnetic field of H = 7 T. No changes in the x-ray spectra (at the same temperatures) were observed without and with the magnetic field (see, for example, the spectra at T = 4.2K in Fig. 1).

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