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Neutron Scattering Study of Hydrogen in Copper[1] ALEXANDER I. KOLESNIKOV, Oak Ridge National Laboratory, VLADIMIR E. ANTONOV, Institute of Solid State Physics RAS, Chernogolovka, Russia, GARRETT E. GRANROTH, Oak Ridge National Laboratory, VALERY I. KULAKOV, MICHAIL A. KUZOVNIKOV, Institute of Solid State Physics RAS, Chernogolovka, Russia, KEN C. LITTRELL, EUGENE MAMONTOV, Oak Ridge National Laboratory — Until now, vibrational spectra of hydrogen in the group 1b metals, Cu, Ag and Au, have never been investigated. Meanwhile, these elements are often used in hydrogen containing atmospheres, therefore the properties of hydrogen in these metals are of significant interest. For the present study, Cu-H samples were synthesized by exposing bulk copper to a hydrogen gas at a pressure of 7 GPa and T=900 K and recovering the samples to ambient conditions. The samples were studied by inelastic (INS), quasielastic and small angle neutron scattering. Nearly all hydrogen (∼10 at.%) contained in the samples proved to be in the form of H2 molecules trapped in large (>>100 A) pores/bubbles in the copper matrix. Para <=> ortho transitions in these molecules give intense peaks at +-14.4 and 28.8 meV in the INS spectra. On heating the sample, the molecular hydrogen melts in a temperature interval from 14 to 60 K corresponding to the gradual increase in the H2 pressure in the pores from 5 bar to 3 kbar. A small narrow peak at 73 meV is also observed in the INS spectra. The peak can only be assigned to a local mode of a 0.03 at.% H impurity in the copper bulk. This is the first observation of H vibrations in a group 1b metal.

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