Zero-field NMR, Mössbauer effect and neutron diffraction in $CuFeS_2$

Gainov R.R.[1,2], Golovanevskiy V.A.[3,4], Vagizov F.G.[1], Khassanov R.R.[1], Douglav A.V.[1], Nemkovskii K.[5], Prokes K.[2], Yokaichiya F.[2], Russina M.[2]

[1]Kazan Federal University, Kazan (Russia)
[2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin (Germany)
[3]Curtin University of Technology, Kent St., Bentley, Perth (Australia)
[4]Tomsk Polytechnic University, Tomsk (Russia)
[5]Forschungszentrum Jülich GmbH (JCNS), Jülich (Germany)
g_ramil@mail.ru

Recent low-temperature studies of antiferromagnetic semiconductor $CuFeS_2$ with $T_N = 823$ K by NMR and Mössbauer effect have revealed the second-order phase transition around 50 K [1]. Antiferromagnetism is caused by Fe electronic spins. The transition observed is connected, likely, with Cu electronic spins having quite small magnetic moments (less than 0.05 μ_B), which is in agreement with previous powder neutron diffraction results [2, 3]. On the other hand, the nature of the low-temperature magnetic state of chalcogenides in general is still unclear. For example, XAFS investigation points to the lack of influence of Cu spins on the phase transition at 50 K [4]. As result, preliminary neutron diffraction studies of a unique single-crystal sample of natural $CuFeS_2$ have been carried out at low temperatures in order to clarify the previous data for powder samples, including structural and valence state properties. The single-crystal neutron diffraction data is preferable to that of the powder samples because of the gain in the Bragg peak intensities. First results prove the presence of the 50 K phase transition. The character of the temperature dependence points to the structural transformations, which influence on the behavior of electronic spins. The report presents the results of experimental studies of chalcopyrite $CuFeS_2$ and a discussion of the observed electronic and magnetic properties.

This work is supported partly by the project BMBF-05K12CB1.

REFERENCES

1. *Golovanevskiy V.A.* Low-temperature Mössbauer and NMR spectroscopy studies of selected Cu-Fe-S chalcogenides / V.A. Golovanevskiy, R.R. Gainov, V.V. Klekovkina, F.G. Vagizov, et al. // Conference proceedings ICAME-2013, Croatia. – 2013. – P.28.

2. *Donnay G.* Symmetry of magnetic structures: magnetic structure of chalcopyrite / G. Donnay, L.M. Corliss, J.D.H. Donnay, N. Elliot, J.M. Hasting // Phys. Rev. – 1958 – V. 112. – № 6. – P. 1917-1923.

3. *Woolley J.C.* Low temperature magnetic behaviour of $CuFeS_2$ from neutron diffraction data / J.C. Woolley, A.-M. Lamarche, G. Lamarche, et al. // J.M.M.M. L62. – 1996. – P. 347-354.

4. *Lovesey S.W.* Acentric magnetic and optical properties of chalcopyrite ($CuFeS_2$) / S.W. Lovesey, K.S Knight, C. Detlefs, S.W. Huang, V. Scagnoli, U. Staub // J. Phys.: Condens. Matter. – 2012. – V. 24. – P 216001.