

Результаты распределения химических элементов и спектр распределения элементов в метеорите Царев составил: кислород - 24.13 %; магний - 2.71 %; алюминий - 3.28 %; кремний - 7.82 %; калий - 1.33 %, кальций - 0.59 %; железо - 60.14 % (вес.).

Обычно у каменных метеоритов толщина внешней коры плавления составляет десятые доли миллиметра. Внешние зоны пористые размером от 5 до 20 мкм, количество пор достигает 45%. Поры круглые, закрытые, размером сотые и тысячные доли миллиметра.

Внутренняя структура представляет собой упорядоченные дендритные кристаллы, которые сформировались при остывании, средний размер кристаллов 500 нм.

Работа выполнена при финансовой поддержке Министерства образования и науки Российской Федерации (базовое финансирование по проекту № 3451) и Правительства Российской Федерации, Акт 211, Соглашение № 02.А03.21.0006.

1. Витязев А.В., Печерникова Г.В., Сафронов В.С. Планеты земной группы: Происхождение и ранняя эволюция. М.: Наука. Гл. ред. физ.-мат. лит., 296 с (1990).
2. Додд Р.Т. Метеориты: Петрология, Геохимия. М.: Мир, 384 с. (1986).

SPIN S=1 CHAIN MODEL FOR BaMoP₂O₈

Badrtdinov D.I.^{1*}, Hembacher J.², Mazurenko V.V.¹, Tsirlin A.A.²

¹) Ural Federal University, Yekaterinburg, Russia

²) University of Augsburg, Augsburg, Germany

*E-mail: reason2205@yandex.ru

Low dimensional systems attract a lot of attention due to formation of nontrivial magnetic orders such as spin-spiral and spin liquid states, skyrmion lattices, etc. The system BaMoP₂O₈, having the monoclinic C2/m space group, is suggested to be quasi-two-dimensional (2D), where molybdenum atoms form triangular lattice [1].

Within this work the powder sample of BaMoP₂O₈ was synthesized, thermodynamic measurements revealed the formation of long range magnetic order with Neel temperature T_N ~ 21K. Further investigation by neutron diffraction experiment identified the magnetic reflection at 17.5°, which obeys to magnetic symmetry with propagation vector $\mathbf{k} = (1/2, 1/2, 1/2)$. The value of magnetic moment 1.48μ_B decreases with increasing temperature, finally disappearing at T_N = 21.4K (Fig.1).

As for theoretical part, density functional calculations within generalized gradient approximation (GGA) elucidate the energy bands near the Fermi level, which corre-

spond to the $\text{Mo}(t_{2g})$ states hybridized with $\text{O}(p)$ states. Using Wannier functions as a basis for construction of low energy states near the Fermi level, we evaluated magnetic form-factor and performed refinement procedure of the neutron diffraction spectra. Taking correlation effects into account within GGA+U method, we estimated individual exchange integrals for our magnetic model. Interesting to note that these calculations give us quasi-one-dimensional chains with main exchange integral $J_2 = 4.6$ meV. This model differs from expected 2D picture, which we concluded from the analysis of crystal structure. Constructed chain model was solved within quantum Monte Carlo (QMC) approach, and obtained magnetic susceptibility shows qualitative agreement with experiment (Fig.1). The maximum of curve is shifted to 20 K, which might be result of the presence of quantum fluctuations and magnetic frustrations, realizing in BaMoP_2O_8 [2].

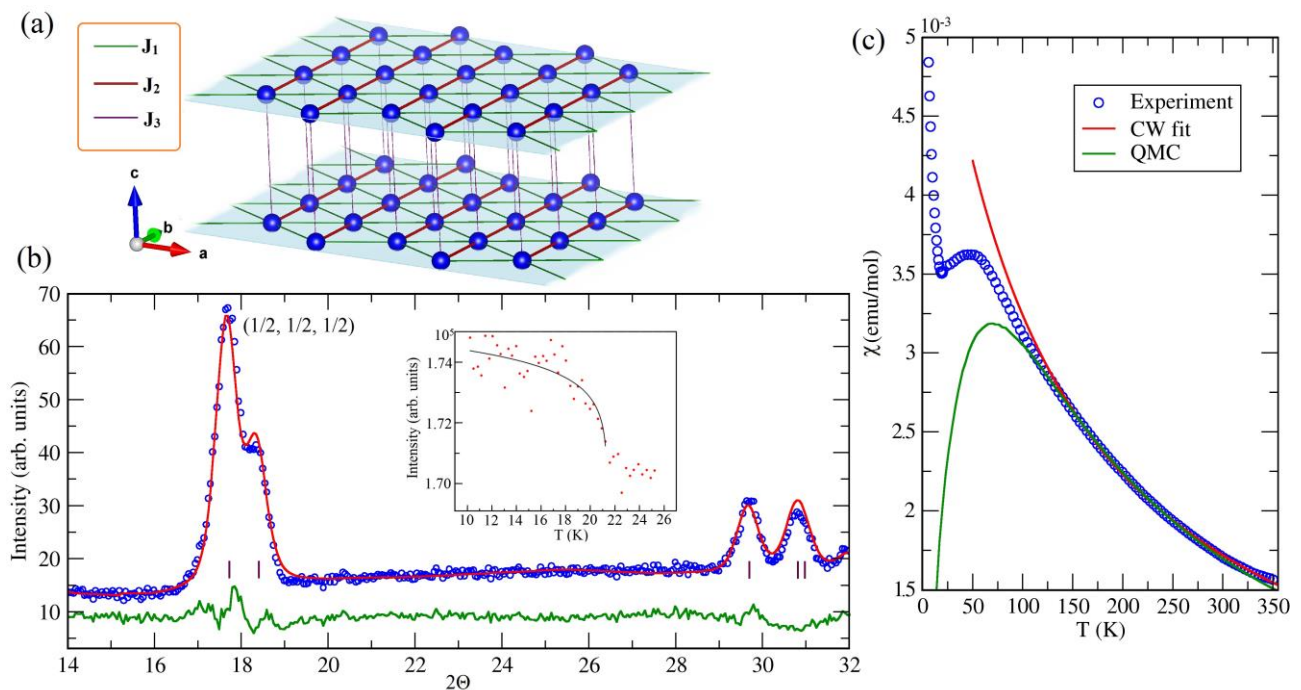


Fig. 1. (a) Constructed magnetic model of BaMoP_2O_8 ; (b) The spectra of neutron diffraction experiment (blue circles) measured at 1.5 K after subtracting the paramagnetic background of 30 K and refinement result (red line). The insert shows the dependence of magnetic reflection on temperature; (c) Experimental magnetic susceptibility in comparison with theoretical approximations.

The reported study was funded by RFBR according to the research project № 18-32-00018

1. Leclaire A. et al., Journal of Solid State Chemistry 116, 364 (1995).
2. Irkhin V.Yu., Katanin A.A. Phys. Rev. B 55, 12318 (1997).