**MS35-P1** **Diffraction methods for detailed studies of the Dzyaloshinskii-Moriya ferroics** Vladimir E. Dmitrienko,[a] V. A. Chizhikov,[a] E. N. Ovchinnikova,[b] G. Beutier,[c] S. P. Collins,[d] G. Nisbet,[d] Y. O. Kvashnin,[e] *[a]Institute of Crystallography, Moscow, Russia, [b]Physical Department, Moscow State University, Russia [c]SIMaP, CNRS—Grenoble-INP—UJF, France, [d]Diamond, Harwell Science & Innovation Campus, UK, [e]ESRF, Grenoble, France.*
E-mail: dmitrien@crys.ras.ru

The Dzyaloshinskii-Moriya (D-M) spin-orbit interaction is an important coupling mechanism between ferroelectricity and magnetism in multiferroics [1]. Therefore it is interesting to find novel methods for quantitative studies of this interaction including its relation with crystal and electronic structure. Specifically, such methods would allow detailed comparison with available theoretical predictions based on *ab initio* simulations. After an introductory survey, two examples of recent development will be presented in detail. First, different experimental techniques sensitive to the *sign* of the D-M interaction are discussed: neutron diffraction, Mössbauer γ-ray diffraction, and resonant x-ray scattering. In all these cases, the sign can be determined from interference between magnetic and structural scattering (resonant and non-resonant) [2] and can be calculated from the first principles [3]. The techniques discussed have their advantages and drawbacks. Classical examples of antiferromagnets with weak ferromagnetism ($FeBO_3$ and hematite, $\alpha$-$Fe_2O_3$) are considered in detail. Recent experimental determination of the D-M sign in $FeBO_3$ using resonant x-ray scattering and comparison of this result with *ab initio* simulations will be also presented. Another example deals with chiral structures in ferromagnetic and multiferroic materials with the space group $P2_13$ (MnSi, $Cu_2OSeO_3$, *etc*.). It is shown how the wave vector and the sign of magnetic helices can be related with the D-M vectors of interatomic bonds [4]. Symmetry analysis of the D-M interaction reveals a non-trivial antiferromagnetic pattern of tilted Mn moments in MnSi remaining even after unwinding of the ground-state helix by the strong magnetic field. It is shown [5] that the tilting can be observed via pure magnetic reflections in neutron or x-ray magnetic scattering. In addition, the D-M-induced antiferromagnetic ordering could be important for the Skyrmion structures, for the spectra of magnetic resonances, and for a better understanding of magnetism-structure interplay in ferroics. This work was supported by the RFBR Grant No. 10-02-00768 and by two projects of the Presidium of the Russian Academy of Sciences: "Thermophysics and Mechanics of Extreme Energy Actions and the Physics of a Strongly Compressed Substance" and "Diffraction of Synchrotron Radiation in Multiferroics and Chiral Magnetics".

[1] Cheong, S.-W. & Mostovoy, M. (2007). *Nature Mater*. **6**, 13-20.
[2] Dmitrienko, V. E., Ovchinnikova, E. N., Kokubun, J., & Ishida, K. (2010). *Pis'ma Zh. Eksp. Teor. Fiz*. **92**, 424 [*JETP Lett*. **92**, 383-387].
[3] Katsnelson, M. I., Kvashnin, Y. O., Mazurenko, V. V., & Lichtenstein, A. I. (2010). *Phys. Rev. B* **82**, 100403.
[4] Chizhikov, V. A. & Dmitrienko, V. E. (2012). *Phys. Rev. B* **85**, 014421.
[5] Dmitrienko, V. E. & Chizhikov, V. A. (2012). *Phys. Rev. Lett*. **108**, 187203.

**Keywords: ferroics and multiferroics; resonant x-ray scattering; magnetic neutron scattering**

**MS35-P2** **Structural phase transitions related to magnetic phenomena in $CuCrSe_2$ and $AgCrSe_2$ magneto-elastics.** Anna Gągor[1], Adam Pietraszko[1], L. Gulay[2] *[1]Institute of Low Temperature and Structure Research Polish Academy of Sciences, Okólna 2, 50-422 Wroclaw, Poland [2]Department of Ecology and Protection of Environment, Volyn National University, Voli Ave 13, Lutsk, Ukraine*
E-mail: a.gagor@int.pan.wroc.pl

Ternary triangular lattice dioxides and chalcogenides crystallize in a highly anisotropic layered structures. In these quasi two-dimensional systems the magnetic ions are arranged on triangular sites. This specific geometry introduce magnetic frustrations states that results in complex magnetic structures and multiferroic properties at low temperatures. Particularly, three-dimensional spiral spin structures may induce electric polarization. This, so called "spin driven" ferroelectricity has been revealed in delaffosites as *e.g.* $CuCrO_2$, $AgCrO_2$ [1,2]. Most of the 'spin driven' multiferroics are oxides and the magnetic interactions are mediated by the oxygen atoms, however the role of the ligand in creation of the multiferroic states has not been yet recognized well. The recent neutron diffraction results indicate that sulfur analogs $AgCuS_2$ and $CuCrS_2$ belong to the geometric multiferroics where the electric dipole arises from the lattice distortion induced by the magnetic ordering. Here, we report the magnetically induced structural phase transitions in the $CuCrSe_2$ and $AgCrSe_2$ single-crystals using combined Mo $K_\alpha$ and synchrotron X-ray diffraction. In both materials magnetic susceptibility and specific heat measurements reveal antiferromagnetic anomaly at $T_N$~58 K and in both crystals lattice effects accompanying the transition are observed. $CuCrSe_2$ and $AgCrSe_2$ crystalize in *R*3*m* symmetry. Simultaneously with antiferromagnetic long-range order that sets at $T_N$ there appear a distortion that decrease the symmetry of the crystal structure to monoclinic. Phase transition has an impact on the inter-plane Cu-Cr distances and introduces deformation of the high temperature symmetric Cr-hexagon. The distortion generates three various magnetic exchange paths: nearest-neighbor exchange $J_1$ and next nearest-neighbor $J_2$ in plane of deformed hexagon and inter-layer exchange $J_3$ via Cr-Se-Cu-Se-Cr path. The significant contraction of the Cu-Cr distance through the transition provides the evidence of the important role of the inter-layer exchange in generating magnetic ground state.

**Acknowledgments:** This work was supported by Ministry of Science and Higher Education in the frame of grant No. N N202 260939

[1] Seki, S. et al. Phys Rev Lett. 2008,101,067204;
[2] Kimura, K. et al. Phys Rev B 2008,78,140401;
[3] Singh, K. et al. Ch. Chem. Mater. 2009, 21 5007-5009;
[4] Rasch, J. et al. Phys Rev B 2009, 80, 104431

**Keywords: magneto-elastics, phase transitions, selenides,**