



## Session V, November 21, Thursday

L16

### STRUCTURAL BIOLOGY INFRASTRUCTURES AT SOLARIS SYNCHROTON IN KRAKÓW

Przemysław Grudnik<sup>1,2</sup>, Joanna Sławek<sup>1</sup>, Maciej Kozak<sup>1</sup>, Artur Biela<sup>1</sup>

<sup>1</sup>Jagiellonian University, SOLARIS National Synchrotron Radiation Centre, ul. Czerwone Maki 98, Kraków, Poland

<sup>2</sup>Jagiellonian University, Małopolska Centre of Biotechnology, ul. Gronostajowa 7a, Kraków, Poland

The SOLARIS National Synchrotron Radiation Centre in Kraków is a leading facility for structural biology research. This presentation highlights the key infrastructures available, including the ARYA beamline, Cryo-Electron Microscopy (Cryo-EM) facilities, planned new beamlines, and the Structural Biology Core Facility at the neighboring Małopolska Centre of Biotechnology (MCB).

One of the most anticipated developments at SOLARIS is the ARYA beamline, designed for macromolecular X-ray crystallography. ARYA is expected to be operational by 2027 and will offer a fully automated system capable of high-throughput crystal analysis within the 5-16 keV energy range. The beamline will also support specialized experiments, including high-pressure studies and crystallographic fragment screening, making it a significant enhancement to the current capabilities of SOLARIS.

The Cryo-EM Facility at SOLARIS, established in 2018 and fully operational since 2019, features two advanced cryo-electron microscopes: the Titan Krios G3i and Glacios. These instruments allow researchers to conduct

high-resolution imaging at cryogenic temperatures, supporting various studies in life sciences, biotechnology, and materials science.

In addition to ARYA, SOLARIS is expanding its capabilities with new beamlines like CIRI and SMAUG, which are under construction and will offer additional experimental techniques in the coming years. These expansions will further solidify SOLARIS's role as a premier center for structural biology.

Adjacent to SOLARIS, the MCB hosts the Structural Biology Core Facility (SBCF), providing services essential for protein structure determination. The SBCF supports both X-ray crystallography and cryo-EM projects, offering expert guidance and customized solutions from sample preparation to structure solving.

Together, the facilities at SOLARIS and MCB provide an integrated and advanced infrastructure for structural biology, positioning Kraków as a key hub for structural biology research in this field.

*This lecture was cancelled.*

L17

### MAGNETO-STRUCTURAL PROPERTIES OF Ho<sub>3</sub>Co (AT AMBIENT AND UNDER HIGH PRESSURE)

Srikanta Goswami, M. S. Henriques, V. Petříček, P. D. Babu

*Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic*

$R_3T$  ( $R$  = rare earth and  $T$  = transition metals) type of rare earth rich intermetallic compounds possess highest  $R$  content in the  $R$ - $T$  binary family and exhibit various interesting magnetic properties emerging out of their complex magnetic structures. These compounds crystallize in the orthorhombic crystal symmetry with  $Pnma$  space group. Ho<sub>3</sub>Co is an interesting case, in this family, that has been studied in the present experimental work based on bulk magnetic measurements such as: dc magnetization, specific heat, ac-susceptibility and also microscopically by neutron powder diffraction. Bulk magnetic measurements at ambient condition suggest that the magnetic structure below the Néel temperature at  $T_N$  ( $= 21$  K) changes continuously until another antiferromagnetic (AFM) transition occurs at  $T_i$  ( $= 9$  K). The incommensurately modulated magnetic structures of this compound at different tempera-

tures were solved by magnetic superspace formalism. The magnetic superspace group describing the spin configuration realized in Ho<sub>3</sub>Co explains the evolution of the structures with temperature and supports the speculations drawn from the bulk magnetic measurements. Below  $T_i$ , the magnetic modulation is anharmonic. Further, frequency dependent experiments reveal the coexistence of spin glass like states with non-collinear AFM order at low temperature. Externally applied pressure wipes out the low temperature magnetic transition at  $T_i$ . The AFM interactions are strengthened with increasing pressure at low temperature while the weak signature of spin glass like state remains up to 1.10 GPa.

*This lecture was cancelled.*

## MINERALS WITHIN THE PD-NI-AS SYSTEM: CRYSTAL STRUCTURES

F. Laufek<sup>1</sup>, A. Vymazalová<sup>1</sup>, D.A. Chareev<sup>2</sup>, T.L. Grokhovskaya<sup>3</sup>, V.V. Kozlov<sup>3</sup>, J. Plášil<sup>4</sup><sup>1</sup>Czech Geological Survey, Geologická 6, Prague 5, Czech Republic<sup>2</sup>Institute of Experimental Mineralogy, RAS, Chernogolovka, Moscow, Russia<sup>3</sup>Institute of Geology of Ore Deposits, Petrology, Mineralogy and Geochemistry RAS, Moscow, Russia<sup>4</sup>Institute of Physics ASCR, v.v.i., Na Slovance 2, 128 21 Prague 8, Czech Republic  
frantisek.laufek@geology.cz

There are three ternary phases in the Pd-Ni-As system described as minerals, nipalarsite  $\text{Ni}_8\text{Pd}_3\text{As}_4$ , menshikovite  $\text{Pd}_3\text{Ni}_2\text{As}_3$  and majakite,  $\text{PdNiAs}$ . Majakite and menshikovite were described as new minerals by Genkin [1] and Barkov [2], respectively. Their crystal structures have been hitherto unknown. Nipalarsite was described together with its crystal structure determination by Grokhovskaya et al. [3]. Majakite was found in intergrowths with other platinum minerals in chalcopyrite and thalnakhtite ores of the Mayak mine (Talnakht deposit), menshikovite was discovered in mafic-ultramafic layered complexes Lakkulaisvaara and Chiny, Russia. A fragment of menshikovite extracted from a sample from Lakkulaisvaara intrusion, Russia, was used for a structure analysis of this mineral. As the natural majakite proved to be unsuitable for a structural analysis, crystal structure analysis was carried out on a synthetic analogue  $\text{PdNiAs}$ .

The synthetic analogues of majakite and menshikovite were prepared using the Kullerud's evacuated silica-glass tube method. Pure elements were used as starting materials for synthesis. The evacuated tube with charges were heated at 400 °C for several weeks. The experimental products were rapidly quenched in cold water.

The crystal structure of  $\text{PdNiAs}$ , a synthetic analogue of majakite, was solved from single-crystal X-ray diffraction data and refined to  $R = 6.68\%$ . Synthetic  $\text{PdNiAs}$  shows  $Pnma$  symmetry and  $a = 15.517$ ,  $b = 3.597$  and  $c = 6.017$  Å unit cell. Its crystal structure contains a mackinawite-like blocks of edge sharing  $[\text{NiAs}_4]$  tetrahedra parallel to (001). Palladium shows unusual five-fold coordination resembling a tetragonal pyramid by As atoms. The coordination of Pd is further completed by close contacts with Ni and Pd atoms. Palladium atoms are located in voids between blocks of  $[\text{NiAs}_4]$  tetrahedra. The structural identity between majakite and synthetic analogue  $\text{PdNiAs}$

was confirmed by comparison of electron back-scattered diffraction (EBSD) patterns obtained from natural grains and patterns generated from our orthorhombic crystal structure model. A phase transition from low-temperature orthorhombic phase to the high-temperature hexagonal phase was observed. The hexagonal phase  $\text{PdNiAs}$  was already described by Evstigneeva [4].

Menshikovite crystallizes in  $Cmcm$  space group and shows unit cell parameters  $a = 15.728$ ,  $b = 6.000$  and  $c = 4.955$  Å. Menshikovite crystal structure contains deformed  $[\text{NiAs}_4]$  tetrahedra. Each  $[\text{NiAs}_4]$  tetrahedra shares one edge with one adjacent tetrahedra along the  $a$ -axis and two opposing edges with adjacent tetrahedra along the  $c$ -axis forming chains of edge-shared  $[\text{NiAs}_4]$  tetrahedra running in 001 direction. Nickel atoms have three close contacts with adjacent Ni atoms across the shared tetrahedral edges. Palladium atoms show trigonal bipyramidal coordination by As atoms. The crystal structure of menshikovite also contains number of Ni-Ni and Pd-Ni close contacts.

1. A. D. Genkin, T.L. Evstigneeva, N.V. Troneva, L.N. Valsov, *Int. Geol. Rev.*, **20**, (1976), 96.
2. A. Y. Barkov, R.F. Martin, Y.A. Pakhomovsky, N.D. Tolstykh, A.P. Krivenko, *Can Mineral.*, **40**, (2002), 679.
3. T. L. Grokhovskaya, O.V. Karimova, A. Vymazalová, F. Laufek, D.A. Chareev, E.V. Kovalchuk, L.O. Magazina, V. A. Rassulov. *Min. Mag.*, **83**, (2019), 837.
4. T. Evstigneeva, Y. Kabalov, J. Schneider. *Material Science Forum*, 321-324, (2000), 700.

*This research was supported by the by the Grant Agency of the Czech Republic (project No. 22-26485S).*

*This lecture was cancelled.*