

MS26-P02 | CHEMICAL BONDING AND STRUCTURAL COMPLEXITY IN KNOWN INTERMETALLIC COMPOUNDS $\text{o-Al}_{13}\text{Co}_4$ AND $\text{Al}_{2.75}\text{Ir}_2$

Grin, Yuri (Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, GER)

Investigations on binary compounds of transition metals with aluminum have a long-time history. The crystal structure of $\text{o-Al}_{13}\text{Co}_4$ was reinvestigated 35 years after the first report about the phase [1,2]. The recent crystal structure redetermination reveals a strong disorder in parts of the unit cell. High-resolution diffraction and TEM experiments show a very complex atomic arrangement obviously deviating from the translational symmetry [3]. The similar situation is found also for the phase $\text{Al}_{2.75}\text{Ir}$ first discovered [4] and much later structurally described [5]. Crystal structure reinvestigation revealed an extremely complex crystallographic picture of two modifications with the LT phase being orthorhombic with doubling of the previous cubic unit cell [6]. The reasons for such complexity may be found in the chemical bonding within the crystal structures characterized by an interplay of the strongly polar and non-polar, two-center and multi-center interactions.

[1] R. C. Hudd, W.H. Taylor, *Acta Crystallogr.* 15, 441 (1962).

[2] Yu. Grin, U. Burkhardt, M. Ellner, K. Peters, *J. Alloys Compds.* 206, 243 (1994).

[3] P. Simon, I. Zelenina, W. Carrillo-Cabrera, U. Burkhardt, M. Feuerbacher, P. Gille, Yu. Grin, unpublished results (2019).

[4] R. Ferro, R. Capelli, R. Marazza, S. Delfino, A. Borseese, G. B. Bonino, *Atti Accad. Naz. Lincei, Cl. Sci. Fis. Mat. Nat. Rend.* 45, 556 (1968).

[5] Yu. Grin, K. Peters, U. Burkhardt, K. Gotzmann, M. Ellner, *Z. Kristallogr.* 212, 439 (1997).

[6] Yu. Prots, J. Kadok, M. Schmidt, M. Coduri, V. Fournée, J. Ledieu, Yu. Grin, unpublished results (2019).