

s8.m27.o1 **MgIr, a new Intermetallic Compound with 25-atoms Crystal Structure Solved from Powder Diffraction.** Radovan Cerny,<sup>a</sup> Guillaume Renaudin<sup>a</sup> and Vincent Favre-Nicolin<sup>b</sup>, <sup>a</sup>University of Geneva, 24 quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland, and <sup>b</sup>CEA/Grenoble, 17, rue des Martyrs, F-38054 Grenoble Cedex 9, France.  
E-mail: Radovan.Cerny@cryst.unige.ch

**Keywords: Powder Diffraction; Structure Solution; Intermetallic Compound**

The crystal structure of a new intermetallic compound MgIr having 25 independent atoms was solved from high resolution synchrotron powder diffraction data (SNBL,  $\lambda = 0.50012 \text{ \AA}$ ,  $2\theta = 2.215 - 41.890^\circ$ , step =  $0.0025^\circ$ , sample in a 0.2 mm glass capillary). First 26 observed reflections were used for indexing (DICVOL91):  $a = 18.46948(6)$ ,  $b = 16.17450(5)$ ,  $c = 16.82131(5) \text{ \AA}$ . The structure was solved (s.g. *Cmca*) by the global optimization of a structural model in direct space using the simulated annealing (in parallel tempering mode) and the program FOX [1]. As a cost function, the integrated  $R_w$  factor and the anti-bump function (based in minimal distances Mg-Ir = 2.7 and Mg-Mg = 2.8  $\text{\AA}$ ) weighted 0.55/0.45 were used. In a final run 13 Ir and 12 Mg free atoms were optimized simultaneously (75 degrees of freedom), and the same solution was always found in less than 5 minutes. The structure was refined by the Rietveld method (FullProf.2k, 76 parameters,  $R_{wp} = 0.094$ ,  $\chi^2 = 3.02$ ,  $R_B = 0.056$ ). Measured composition (EDAX)  $\text{Mg}_{52(2)}\text{Ir}_{48(2)}$  agrees well with the refined one. The structural model was independently confirmed by the single crystal X-ray diffraction [2]. The crystal structure of MgIr can be classified as a topologically close-packed phase that is close to the definition of Frank-Kasper phases. The coordination of nearly all atoms has a form of the Frank-Kasper polyhedra. The Ir-Ir interatomic distances in MgIr are in the range of 2.424(4) - 2.667(2), and are the shortest ever observed in an Ir-containing compound.

- [1] Favre-Nicolin, V. and Cerny, R., *J. Appl. Cryst.* **35** (2002) 734-743 see also: <http://objcryst.sourceforge.net>  
[2] Cerny, R., Renaudin, G., Favre-Nicolin, V., Hlukhyy, V. and Pöttgen, R. *Acta Cryst. B*, submitted.

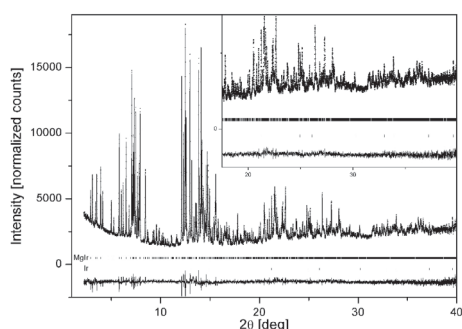


Figure: Rietveld plot for MgIr.

s8.m27.o2 **New Possibilities in Stress and Strain analysis with Synchrotron Radiation and Neutrons.** Anke Rita Pyzalla, TU Wien, Institute for Materials Science and Testing, Wien, Austria, E-mail: [anke.pyzalla@tuwien.ac.at](mailto:anke.pyzalla@tuwien.ac.at)

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Strain and stress analyses using diffraction methods have become increasingly important in the development and characterisation of materials, the optimisation of manufacturing methods (e.g. regarding surface integrity) and the assessment of component behaviour.

Due to the high photon flux and parallelism, synchrotron radiation offers novel possibilities for microstructure, texture and residual stress analyses.

Synchrotron radiation in the medium energy range enables investigations of the phase composition, texture and strain/stress state of the surface region. New possibilities are provided by beam focusing, thus local resolutions up to the sub-micrometer region can be reached.

High energy synchrotron radiation enables microstructure, texture and strain/stress analyses in the bulk of samples. Even in steel samples which have a diameter of several millimetres phase analyses and residual stress analyses can be performed with gauge volumes of only some  $\mu\text{m}^3$  size. Due to the high photon flux analyses with high local resolution and time resolved in-situ analyses become feasible. In future even combined tomography / diffraction experiments may become feasible.

The increasing possibilities for microstructure, texture and residual stress analyses using synchrotron radiation are demonstrated by case studies. These include the surface of worn railway rails, friction stir welds, position and time-resolved in-situ experiments

Neutron diffraction techniques remain important complementary techniques to synchrotron radiation strain/stress analyses especially regarding coarse grained materials as well as components. Examples for experiments using neutrons and synchrotron radiation as complementary techniques are given.