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REFINEMENT OF MAGNETIC STRUCTURES IN JANA2006

V. Petříček and M. Dušek

Institute of Physics of the ASCR, v. v. i., Na Slovance 2, CZ-182 21 Praha 8, Czech Republic
petricek@fzu.cz

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The program Jana is well known system for solution and refinement of regular, modulated and composite crystals. Jana was originally oriented to data collected from a single crystal with a wide support for handling of twinning. In the version Jana2000 the program was generalized for structure refinement from powder data including multiphase option [1]. Finally the multiphase option has been generalized for a single crystal refinement.

During the year 2006 the old code of Jana2000 has been completely rewritten in order to open possibility for adding various new options. Probably the most important change is the option for making joint refinements from different data collections. Thus data sets from powder and single crystal measured with X-rays and neutrons can be used simultaneously.

The magnetic scattering formalism has been implemented recently. The program can be used not only for structures having nuclear and magnetic lattices identical but also for commensurate and incommensurate magnetic and nuclear arrangements. For this reason we have generalized concept of superspace groups, as introduced by Janner, Janssen and de Wolff [2], to magnetic groups. Such an approach has following advantages:

- Simple relationship to the Laue diffraction group facilitates symmetry recognition
- The magnetic structure can be handled even for regularly modulated and composite crystals
- The general modulation wave can account for complicated magnetic modulation – more harmonics, step like modulations, …

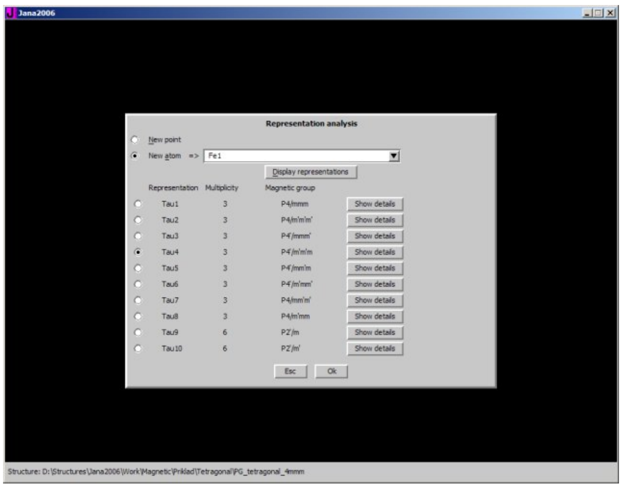

Figure 1. The pilot window for representative analysis for the space group *P*4/*mmm*.

The only disadvantage is that the new formalism may be too complicated for people without an experience with superspace description.

Calculation of magnetic structure factor, which is generally a vector, is based on the general equation:

$$\mathbf{F}_M(\mathbf{h}) = p \sum_i f_i(h) T_i(\mathbf{h}) \mathbf{M}_i \exp(2\pi i \mathbf{h} \cdot \mathbf{r}_i)$$

where p is a normalization constant to transfer magnetic scattering calculated in Bohr magnetos to the scale used for nuclear neutron structure factors, $f_i(h)$ magnetic form factor, $T_i(\mathbf{h})$ is the ADP (temperature) factor and $\mathbf{M}_i$ is the magnetic moment of the i^{th} atom. The geometrical part $\exp(2\pi i\mathbf{h}\mathbf{r}_i)$ is a function of the atom position. Intensity of a magnetic reflection is related to the square length of the magnetic structure factor projected into the reflection plane:

$$I_M(\mathbf{h}) = \mathbf{F}_M^2(\mathbf{h}) - \left|\mathbf{h}/h \cdot \mathbf{F}_M(\mathbf{h})\right|^2$$

The intensity of the magnetic reflection combines with the intensity originating from the nuclear scattering. The combination is made as from independent object (twins):

$$I(\mathbf{h}) = I_N(\mathbf{h}) + I_M(\mathbf{h})$$

The magnetic moments of atoms can follow the same translation periodicity of the nuclear structure or they can have their own periodicity either commensurate or incommen-

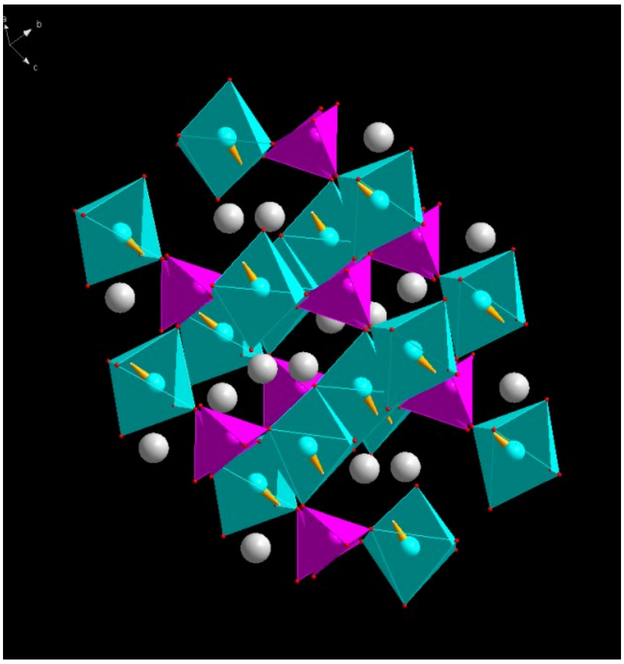

Figure 2. The magnetic ordering for $BiNPO_5$ as refined by Jana2006.

surate with the nuclear lattice. Generally the magnetic moment can be written as a combination of harmonic functions:

$$\mathbf{M}_i(x_4) = \mathbf{M}_{i0} + \sum_{n=1}^{N} [\mathbf{M}_{ins}\sin(2\pi n x_4) + \mathbf{M}_{inc}\cos(2\pi n x_4)]$$

The superspace approach does not give a direct connection to irreducible representation analysis, as introduced by E.F. Bertaut [3]. For this reason we have also implemented a tool which can directly perform such an analysis in the Jana package. This part of the program is analogical to programs such as MODY [4], SARAh [5] and BasIReps [6]. New contribution of Jana is that the result of the representative analysis is transformed (see example in Fig.1) into (super)space magnetic group. Moreover all additional conditions (if any) necessary to assure selected irreducible representation are generated automatically and used during the refinement process. This makes possible to test all acceptable irreducible representation directly in terms of Laue symmetry and systematic extinctions.

The refined magnetic structure can be visualized by calling a suitable external drawing program from Jana2006. In Fig. 2 an example of a refined magnetic structure is drawn by Diamond 3.0 [7].

The program has been already tested on several data sets from different sources (ILL, ISIS, PSI, …). During the lecture more details will be presented about implementation of the magnetic option into Jana2006 and examples of already refined structures will be demonstrated.

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MĚŘENÍ MONOKRYSTALŮ NA PRÁŠKOVÉM DIFRAKTOMETRU

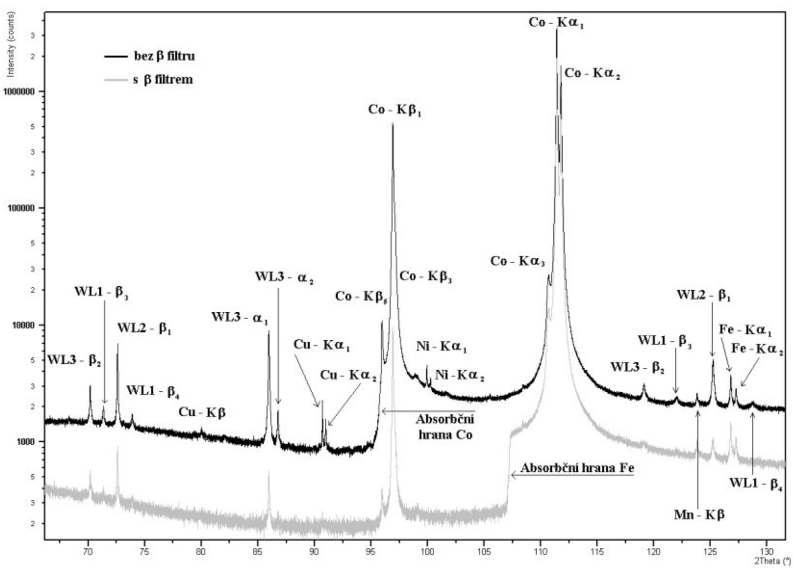
J. Drahokoupil[1,2], J. Kopeček[2]

[1]FJFI ČVUT, Trojanova 13,120 00 Praha 2, ČR
[2]Fyzikální ústav AV ČR, v.v.i., Na Slovance 2, 182 21 Praha 8, ČR
jandrahokoupil@seznam.cz

S monokrystaly se v oblasti práškové difrakce setkáváme velmi zřídka. Při měření práškových dat je jejich výskyt spojen s obavami o výdrž detektoru a s jejich někdy až nečekanými projevy na práškový záznam. V následujících řádcích bude uvedeno několik příkladů měření s monokrystaly a• už s jejich nežádoucím projevem či s jejich záměrným měřením.

V současné profilové analýze je tendence k modelování celého záznamu [1]. Nedílnou součástí této problematiky je i přístrojová funkce. Ta je krom jiného dána i spektrem vlnových délek jdoucích z rtg lampy. Na obr. 1 je uveden difrakční záznam monokrystalu korundu, difraktující rovina 0012 (pro wolframové L-čáry na pravé straně obrázku i 0018) byla rovnoběžná s povrchem. Byl použit divergentní svazek v Bragově-Brentanově uspořádání s geometrií , Co lampa. Jsou zde zakresleny dvě křivky jedno pro měření s a bez beta filtru (Fe).

Taková to měření umožňují popsat spektrum vlnových délek po aplikaci různých optických prvků. Pro profilovou analýzu má v tomto případě největší význam



Obrázek 1. Část difrakční záznamu monokrystalu korundu Al_2O_3. Spektrum vlnových délek a vliv filtru na vlnové spektrum.