Orthorhombic domains in powder RuO2 at ambient conditions

W. Lulka[1*], R. Przeniosło[1], I. Sosnowska[1], F. Fauth[2] and E. Suard[3]

[1]*Faculty of Physics, University of Warsaw, 02-093 Warsaw, Poland*
[2]*ALBA-CELLS BP1413 08290, Cerdanyola del Valles, Barcelona, Spain*
[3]*Institut Laue Langevin, 38042 Grenoble, France*

*e-mail: Wojciech.Lulka@fuw.edu.pl

The crystal structure of the tentative altermagnet RuO_2 was studied by synchrotron radiation based x-ray powder diffraction, constant-wavelength neutron powder diffraction and time-of-flight neutron powder diffraction. The diffraction patterns are best described by Rietveld refinement with the anisotropic Bragg peaks' broadening model. The distribution of the RuO_2 crystallites is composed of a majority of orthorhombic domains (space group *Pnnm*) which coexist with a minority of tetragonal domains (space group $P4_2/mnm$).
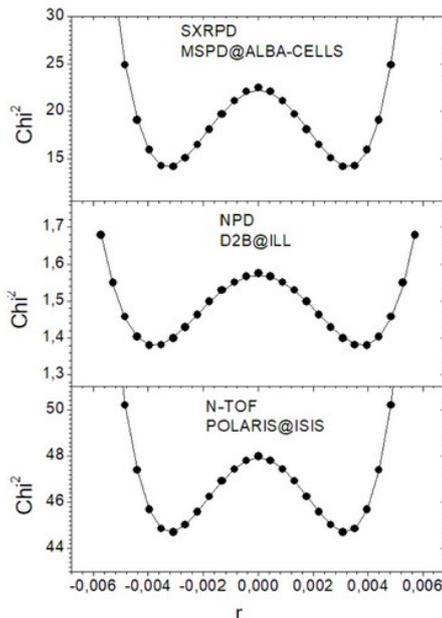
In order to demonstrate the changes of fit quality we have done Rietveld refinements with the orthorhombic symmetry (space group *Pnnm*) for fixed values of the a and b lattice parameters calculated as:

$$a = \langle a \rangle \left(1 + \frac{r}{2}\right); \quad b = \langle a \rangle \left(1 - \frac{r}{2}\right)$$

where $\langle a \rangle$ is the average of a and b obtained in the orthorhombic fit while the orthorhombic deformation parameter r changes between $-0.0057 < r < 0.0057$ with a fixed step. All instrumental, background and structural parameters (except fixed a and b) were refined. Please note that $r = 0$ corresponds to the tetragonal rutile-type fit. The value of $\chi^2(r)$ for the best fit at each value of r is drawn with solid symbols. The curves drawn show the fourth-order even polynomial $f(r) = ar^4 + br^2 + c$ fitted with very good agreement to the observed $\chi^2(r)$ for all three datasets. The results of SXRPD and NPD show good correspondence with each other with a double minimum of $\chi^2(r)$ near r = 0.0036. The neutron diffraction n-TOF pattern measured with a powder RuO_2 sample from a different batch than the first two gives also a clear minimum near r = 0.0032.

References

1. J. Haines, J. M. Leger, O. Schulte, and S. Hull, Neutron Diffraction Study of the Ambient-Pressure, Rutile-Type and the High-Pressure, CaCl2-Type Phases of Ruthenium Dioxide, Acta Crystallographica Section B 53 (1997) 880.