Poster Presentation

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Identifying almost identical phases by 3D electron diffraction

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Magnetically frustrated materials have been the subject of many studies over the last decades. In search for a 3-dimensional quantum spin liquid, where quantum-mechanical fluctuations prevent magnetic order, different phases of stoichiometry Ba3NiSb2O9 have recently [1] been synthesized some of them at high pressure. Two of these phases are hexagonal. The hexagonal phases (space groups P63/mmc and P63mc, respectively) have different structures but cell parameters that differ by less than 1%. Similar phases have been obtained with Cu [2] or Co [3]. These phases are well distinguished by powder X-ray diffraction when they appear in sufficient quantity in a newly synthesized powder. When these phases are present only in minor quantities, which is a common situation when synthesizing new materials, only transmission electron microscopy can give structural information on a very local scale. However, the accuracy of unit cell parameter determination by electron diffraction (usually 1% or worse) and the identical extinction conditions for the 2 space groups don't permit to distinguish between the two phases. Convergent beam electron diffraction could show the difference between the centrosymmetric and non-centrosymmetric space groups provided a suitably oriented particle can be found. In this work we propose a different method of distinguishing structures in such complicated cases by actually solving the structure. Sufficient in-zone axis precession electron diffraction and/or electron diffraction tomography data can be obtained from any crystal regardless of its orientation. In the subsequent structure solution we have tested both space groups. The quality (or absence thereof) of the structure solutions obtained clearly makes it possible to distinguish between the two hexagonal structures.

[1] *J.G. Cheng, G. Li, L. Balicas et al., Phys. Rev. Lett., 2011, 107, 197204,* ***[2]*** *S. Nakatsuji, K. Kuga, K. Kimura et al., Science, 2012, 336, 559-563,* ***[3]*** *Y. Doi, Y. Hinatsu and K. Ohoyama, 2004, J. Phys.: Condens. Matter, 16, 8923-8935*

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