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Phase Identification by Rotation Electron Diffraction from Multiphasic Samples

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Electron Crystallography is an important technique for studying micro- and nano-sized crystals[1]. Crystals considered as powder by X-ray diffraction behave as single crystals by electron diffraction. Recently we developed a new method, Rotation Electron Diffraction (RED) for three-dimensional diffraction data collection by combining electron beam tilt with goniometer tilt on a transmission electron microscope (TEM)[2]. Here we apply the RED method on an unknown oxide sample in a Ni-Se-Cl-O system, which may show special physical properties, for example magnetic properties. The crystals in the sample were less than a few micrometers in sizes. Powder X-ray diffraction patterns of the sample could not be indexed by existing known phases. The sample was thus studied by TEM. Five 3D RED datasets were collected from five crystals with different morphologies using the software package RED. The data processing was also performed using the software RED-processing. The unit cell and space groups of all the five phases were obtained using RED and the structures of four of five phases were solved. Nearly all peaks in the powder X-ray diffraction pattern could be indexed using these five phases. To conclude, five phases from a powder sample have been identified using RED. RED is a powerful method for phase identification of multiphasic samples with nano-sized crystals.

[1] Zou X.D., Hovmöller S., Oleynikov P., *IUCr Text on Crystallography*, Oxford University Press, 2011., [2] Zhang D.L., Oleynikov P., Hovmöller S., et al., *Z. Kristallogr.* 2010, 225, 94-102.

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