MS25-P06 | Low Dose Electron Diffraction Tomography (LD-EDT) solves the structure of a new $(Na_{2/3}Mn_{1/3})_2Mn_3Ge_3O_{12}$ phase synthesized at high pressure and high temperature

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Our team has recently developed the LD-EDT method [1], which makes it possible to study the crystallographic structure of sensitive materials that are very promising in many fields (medical, energy, etc.), but from which one cannot obtain single crystals large enough for X-ray diffraction. The LD-EDT method, based on electron diffraction tomography, eliminates all periods of irradiation of the sample except those actually used for data acquisition. It therefore uses the minimum dose (< 1 electron/A^2). In addition, the LD-EDT method ensures that the diffracting volume of the crystal remains the same at all stages, which leads to particularly reliable data.

We present here the structure solution of a new sodium compound, discovered in a polyphase powder, synthesized under high pressure and high temperature in the framework of expanding the range of germanium-based compounds in the pyroxene family. Since it is well known that sodium migrates or vaporizes under the electron beam, we decided to apply the new LD-EDT method to acquire the diffracted intensities without damaging the crystals. The structure was solved by direct methods: $(Na_{2/3}Mn_{1/3})_2Mn_3Ge_3O_{12}$ crystallizes in a (*Ia-3d*) garnet-like cubic structure, with a cell parameter of 12.0 Å. The refinement against X-ray powder diffraction data revealed a mixed Na/Mn occupancy on one site.

[1] Stéphanie Kodjikian and Holger Klein, Ultramicroscopy 200 (2019) 12-19