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Experiment Report Form

ESRF	Experiment title: Detailed structure of impact diamonds from Popigai meteorite crater by µm-beam X-ray diffraction	Experiment number : ES-362
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The aim of the project was an investigation of structure and composition of inclusions in impact diamonds as well as characterisation of the diamond matrix by μ m-beam X-ray diffraction and photoelectron spectroscopy. We investigated 10 crystals of 240-400 μ m collected and preliminary characterized using *in house* single crystal diffractometer equipped with a microfocus Cu X-ray tube. 28 particles from the 60-100 μ m fraction were collected on site based on their shape and colour. All particles have plate-shape and were fixed to the SiN membrane for further mapping. Based on our previous experience, we conclude that investigated particles are representative for whole massive and can be used for the modelling of properties and structure characteristic for impact diamonds in general.

All diamond particles (both, larger fraction with inclusions visible using *in house* techniques as well as crystals collected on site according to their colour) have similar properties with large variations of inclusions dimensions. All particles contain small 1-5 μ m inclusions, which cannot be investigated using alternative techniques. Fe, Cr, Ni, Cu, Zn, Ti, Ca, K and light elements (such as Al, Si, S, Cl) were detected in inclusions. Traces of heavier elements such as Tl, Pb and Ce were also detected (Figure 1).

The following phases have been suggested according to their diffraction characteristics: Fe_4C , $Ca/SrTiO_3$, *bcc*-(Fe,Cr,Ni) alloy, $CaCO_3$ (calcite), SiO_2 (quarz), Fe_2O_3 . Some of inclusions are quite unusual for impact diamonds and have never been described in the literature. High spatial and diffraction resolution allow us to detect inclusion phases perfectly masked by the diamond matrix.



Figure 1. Distribution of 1^{st} raw transition elements over a diamond particle according to XRF data: (a) Fe-Cr, (b) Fe-Ni, and (c) Fe-Cu plots. Fe shown in red channel, integral X-ray fluorescence in blue, Cr, Ni, Cu – in green. Scan height and wide dimensions are of 240 μ m.

As our primary interests were focused on the diamond matrix, inclusion-free areas were investigated to obtain diffraction patterns suitable for quantification Lonsdaleite admixture and characterization of diamond's defect structure. The matrix is quite uniform along all crystals. It should be noted, that each crystal shows all features characteristic for defect diamond's structure. The middle parts of crystals show diffraction patterns typical for powdered samples or superposition of a number of simple defect diamond domains. Outer ranges have isolated wide spots and stripes characteristic for a cubic diamond with defects.

1D diffraction patterns reconstructed from the frames obtained for inner areas can be interpreted as cubic diamond with an admixture of hexagonal Lonsdaleite phase. Nevertheless, outer parts do not show any reflexes characteristic for hexagonal diamond as well as we did not obtain any areas with pure Lonsdaleite. It can be a proof for the complexity of structural defects where classical models with planar defects cannot be applied. More intricate models should be applied to explain diffraction patterns. At the moment, we are looking for more adequate models using theoretical modelling of individual crystals and transmission electron microscopy.



Figure 2. Diffraction data for inner part of one-domain defect diamond particle: (a) experimental frame, (b) azimuthal (2D) and (c) XPD-like (1D) pattern reconstructions. Lonsdaleite defects give arc-like bands on azimuthal patterns.