Poster Presentation

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Single crystal diffraction at high energy and high pressure on I15 at DLS

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The Extreme Condition beamline (I15) at the Diamond Light Source is a dedicated beamline for powder as well as single crystal diffraction on samples at extreme conditions in pressure or temperature. Single crystal data on either pressurized samples in a diamond anvil cell (DAC) or at ambient conditions are routinely done on a diffractometer scanning ϕ and ω using X-rays with energies in the range from 20 keV to 80 keV. Depending on the sample beam sizes varying from 20 µm to several 100 µm can be used. Data are recorded with an Atlas CCD (Agilent Technologies) and then treated with the Crysalis software package. In this contribution we highlight the very high accuracy of single-crystals data obtainable at I15 on two examples of single crystals in a DAC (E = 40 keV) and a sample at ambient conditions (E = 60 keV). A single crystal of the binary transition metal compound FeGe (B20 structure, space group P213, Z=4) was studied up to 11 GPa to determine the evolution of the inter-atomic distances (both atoms occupy the 4a Wyckoff positions). More than 200 unique data could be used to refine 7 parameters with an average R1 on all data of ~7%. Very high quality data have also been obtained for single crystals from the field of chemical crystallography, for which not only connectivity but also small bonding features can be detected. For example in l,6;8,13 biscarbonyl[14]annulene the progressive loss of aromatic character could be monitored and, in a special setup, the data allowed for the refinement of an unconstrained multipolar model. The use of 60 keV photons was crucial for an experiment on natural diamonds containing a variety of inclusions. At these energies the absorption of the diamond can be neglected. The aim of the study was to obtain information on possible recurrent crystallographic relationships between the inclusions and the diamond host on a significant number of extremely rare natural diamonds containing minerals.

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