

intense X-ray pulses with matter. Some of the results obtained so far, including the first steps towards single particle imaging, will be presented. The FLASH results strongly support the high expectations for revolutionary science from hard X-ray FELs.

Keywords: synchrotron radiation, free electron lasers, ultrafast dynamics

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Structure refinement and structure modelling: A chemical probe for complex mineral groups

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Minerals usually show widespread solid-solution of many chemical species in a number of structural sites. In rock-forming minerals, cation site-preference and partitioning (when allowed by the crystal structure) depend on both bulk composition and system parameters such as pressure, temperature and water activity, so that cation ordering patterns provide important clues on the evolution of petrogenetic processes. Cation order in a given sample can be inferred by structure refinement (SREF) and supported by spectroscopic analysis; far more reliable results are obtained by comparison with crystal-chemical models based on many solid-solution terms. Surprisingly reliable results can also be obtained via statistical analysis of representative databases built up with a multi-analytical approach including SREF and in situ analysis of all the chemical constituents (H, Li, Be, B included, if relevant to the crystal-chemistry of the mineral group). In the case of the amphiboles, detection and quantification of even elusive constituents such as Li and the oxo component, as well as calculation of the crystal-chemical formula, can now be addressed based only on combination of subtle changes in the geometric and electronic descriptors derived from SREF. Also, reliable regression equations now relate the crystal-chemical formula with unit-cell parameters. They can be used to check the composition of small synthetic crystals (often off composition with respect to the reagents), where in situ analysis is impossible and the only available evidence is powder diffraction analysis. They also provide clues for the non-existence of some particular composition, among which many theoretical end-members. Examples will be given focussing on the crystal-chemistry of amphiboles and garnets.

Keywords: crystal structure databases, single-crystal structure analysis, mineral crystal-chemistry