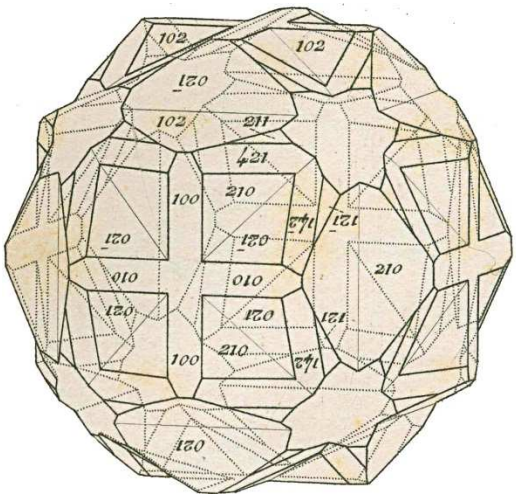

Impact of Crystallography on Modern Science

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Probing the crystal structure of minerals from room to extreme conditions: the contribution of X -ray diffraction in the lab

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Crystallographic researches on materials under extreme conditions of pressure and temperature have been very fashionable topics in the last decades. It is indeed part of the deep inclination of researchers to investigate and understand processes in nature, especially when mechanisms describing changes in the material are strictly related to changes in the structure of crystalline materials. As long as the interest is focused on geological processes, minerals – or their synthetic equivalents – take the leading role. However, the understanding pouring out from crystallographic research on minerals vastly extends in the material science field and ends up enlightening important technological and engineering advances (e.g. zeolites).

When we investigate minerals that we found at the Earth's surface we observe a great deal of phases that have grown at higher temperatures and pressures. Yet, diffraction experiments at ambient conditions tell us very little about how minerals behave in the geological scenarios from they are coming. Technological development has allowed researchers to reach pressure and temperatures very close to Earth's core, in particular when synchrotron light sources are used. The latter allows to access to diffraction data on very small crystal volumes or, by instance, even use energy-dispersive diffraction mode allowing for faster data collection on limited diffraction angle devices required to reach extreme pressures. It would seem therefore useless to keep in-house X-ray diffraction with limited brightness in angle-dispersive diffraction mode with respect to the synchrotron radiation. Notwithstanding, when accessing to large scale facilities time for collecting complete structural data from single crystals diffraction experiments is still very limiting, in particular when it is necessary to follow the mechanism ruling a particular transformation process.

Furthermore, the increasingly better performance of in-house X-ray sources and detectors are closing the gap with respect to large scale facilities regarding diffraction of small crystals. When time and precision is the crux of the problem, X-ray single crystal diffraction in-house still makes the difference. The new generation of in-house X-ray source (Mo or Ag micro source) combined with special optics and detectors only used at large scale facilities so far (see for example the Pilatus 200 and 300 K detectors, which do not have any intrinsic noise) allow to solve and refine the crystal structure of crystals down to even 4-5 microns in size. These systems allow to collect complete intensity data in 20-25 minutes for 40-50 microns in size and just 1-2 hours for extremely small crystals. This opens totally new scenarios in crystallography especially for those synthetic or natural crystalline materials whose crystal sizes are in general not suitable for conventional in-house instruments.