Contribution ID: **86** Type: **Oral contribution**

Experimental Charge Densities of Minerals under Pressure

Tuesday 16 March 2021 15:55 (20 minutes)

This is quite a paradox that a century after introduction of the spherical Independent Atom Model (IAM, 1914 [1]), 99.7% of all ca. 1.5mln known crystal structures, including almost all structures of minerals, have been refined using IAM which suffers from severe methodological deficiencies. Far better results can be obtained when new approaches of quantum crystallography ustilising aspherical atomic factors are applied.
A short beam wavelength (0.4Å) and a special type of Diamond Anvil Cell (DAC) with large opening angle allow us to collect data with extremaly high resolution and 100% completeness up to as high resolution as ca. 0.4 Å.
We will present details of aspherical Hansen-Coppens pseudoatom refinement of electron density which we applied in multipole modeling [2] of electron density in crystals of minerals including minerals under pressure. We have successfully refined quantitative experimental electron densities for crystals of several minerals such as fluorite, grossular and hsianghualite and others. We will present the most interesting results such as onset of F···F interactions (charge-shift bonding) in fluorite [3] and flow of charge among ions in the structure of hsianghualite, Ca3Li2(Be3Si3O12)F2, under pressure. Up to our best knowledge, these are the very first successful experimental determinations of quantitative charge density distributions in mineral crystals under high pressure. They allow for quantitative characterisation of electron density in crystals of minerals including studies of changes of electron density under pressure.
Such studies open a new field of mineralogical subatomic investigations (at the level of changes of electron density properties) of different mineralogical processes in the Earth mantle by simulating them in DAC in laboratory conditions.
KW acknowledges a financial support within the Polish National Science Centre (NCN) OPUS17 grant number DEC-2019/33/ B/ST10/02671.
References:
[1] Compton, A.H., (1915) Nature., 95, pp. 343-344.
[2] Hansen, N. K., & Coppens, P., (1978) Acta Cryst., A34, 909–921.
[3] Stachowicz, M., Malinska, M., Parafiniuk, J., &Woźniak, K., (2017) Acta Cryst., B73, 643–653.
[4] Gajda, R., Stachowicz, M., Makal, A., Sutuła, S., Parafiniuk, J., Fertey, P., & Wozniak, K., (2020) IUCRJ, 7(3), 383-392.

Primary author: WOZNIAK, Krzysztof (University of Warsaw, Poland)

Presenter: WOZNIAK, Krzysztof (University of Warsaw, Poland)

Session Classification: Extreme/non-ambient conditions

Track Classification: Extreme/non-ambient conditions