Ultra-high Resolution Data for Charge Densities Studies

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X-ray diffraction is at present the main experimental technique to obtain the electron density distribution in crystals. Use of the new advanced area detectors allows measuring the ultra-high resolution data almost routinely. Speed of data collection and its quality is optimized when an integrated system for data collection, reduction and structure solution is used. The presented system allows for immediate control of the data quality in terms of such parameters as diffraction limit, completeness, and redundancy during the experiment. The experiment simulation module may minimize the influence of profile overlap and detector obstructions on data completeness. The further optimization can be accomplished by the use of specifically adjusted oscillation angle for each scan. The precise determination of diffraction intensities in the resolution shells between 0.7Å and 0.38Å is achieved by separate treatment of $K_{\alpha 1}$-$K_{\alpha 2}$ split. The ultra-high resolution, high quality data allow for precise analysis of interactions continua for all pairs of interacting atoms. The application of this approach to several systems will be presented.

Keywords: charge density, data collection, $K_{\alpha 1}$-$K_{\alpha 2}$ split