

W0316

Data Collection Strategy and Simulation for High Resolution Experiments. M. Chruszcz¹, M. Cymborowski¹, A. Gawlicka-Chruszcz², Z. Otwinowski³, W. Minor¹, ¹Univ. of Virginia, Charlottesville, VA 22908, ²HKL Research Inc., Charlottesville, VA 22903, ³UT Southwestern Medical Center at Dallas, Dallas, TX 75390.

An approach that integrates data collection, data reduction, and structure solution not only significantly accelerates the process of structure determination but also improves the structure quality. The integrated system allows for fast indexing of the diffraction image, estimating of the effective mosaicity, and calculating of a suitable data collection strategy to achieve maximum data completeness. Usually the strategy programs calculate completeness in an ideal situation that does not take into account beam stop or cooling system obstructions. We present here the system that uses the experiment simulation to calculate the completeness of unique and anomalous data. The simulation takes into account blind regions, including regions generated by moving parts (kappa or eulerian goniostats). The shape and curvature of the detector is also taken into account. In order to minimize the problem of profile overlap, each scan can be performed with a specifically adjusted oscillation angle. The system can be easily adapted to multi-crystal experiments.