An application of multigrain approaches to the structural solution of grains from polycrystalline samples

The overlap of diffraction spots from different grains was investigated to understand the influence of experimental factors on the x-ray diffraction data quality and to optimize the experimental parameters for data collection on polycrystalline samples. Diffraction patterns for photoactive polycrystals were indexed and sorted with respect to grains using multigrain approaches. The indexing of diffraction spots and the identification of grains for tetrathiafulvalene-p-chloranil samples were performed using the ImageD11, GrainSpotter, GRAINDEX and Cell_now programs. In many cases, comparison of the results from these programs shows good agreement. For the individual grains from polycrystalline samples, the crystal structure was solved and refined using the SHELXTL program. After the structural refinement of the grains, the best and the average R1 values were 1.93% and 2.06%, respectively, which are on a comparable resolution level with that obtained from the x-ray single crystal measurements.

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