Calculation of Two-Dimensional Scattering Patterns for Oriented Systems

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A versatile procedure to calculate two-dimensional scattering patterns of oriented systems is presented. The systems are represented by a set of dummy atoms with different scattering length densities which allows the construction of very complex shapes either for single particles or for sets of particles. By the use of oriented pair distances distribution functions it is possible to perform a fast calculation of the scattering intensity from the oriented system in a given direction in the scattering vector (q) space and generate the 2D scattering pattern on a given q plane. Several examples of the calculations are presented (proteins, nanoparticles, supramolecular structures, etc), demonstrating the method and its applicability. Applications in the study of liquid crystals and its internal structure, dimensions and organization will be shown. The presented results open new possibilities for the analysis of scattering patterns obtained from oriented systems [1,2].


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