X-ray structural analysis of soft materials

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The fundamentals of theory and methods of X-ray structural analysis of soft matter (non-crystalline materials, liquids, solutions and amorphous materials) [1] will be presented. The present day state of studies in the field will be discussed and the significance of X-ray structural studies of molecular liquids [2] and nanocarbon systems [3] for the understanding of the mechanism of physico-chemical processes taking place in these materials will be indicated. The significance of crystallography in contemporary X-ray structural analysis of soft matter [4] will be pointed out.

X-ray diffraction is a very efficient method of studying the structure of matter in both solid and liquid phase [5]. Recently [6] it has been shown that the X-ray diffraction method on liquid media allows not only determination of interatomic distances in a molecule but also brings information on the kind of interaction among the molecules and degree of their ordering.

Structure of soft matter (non-crystalline materials, liquids, solutions and amorphous materials) can be described by the radial distrubution function (RDF). The RDF may be represented as a sum of the Gaussian functions [7]:

$$4\pi r^2 \sum_{i=1}^{n}\sum_{j=1}^{n} \overline{K}_i \, \rho_j(r) = \sum_{i,j}^{n} 2\,\overline{K}_i \overline{K}_j \left(\pi\,\sigma_i \sigma_j\right)^{-1/2} \cdot \exp\left[-\left(r - r_{ij}\right)^2 \cdot \left(\sigma_i\,\sigma_j\right)^{-1}\right], \qquad (1)$$

where r_{ij} is the interatomic distance inside a molecule, σ_i and σ_j are the standard deviations of position atoms, which can be expressed as a function of the covalent radii of i and j atoms. By changing the internuclear distances r_{ij} we can get the best fit of the model function (1) to the experimental function. Accurate determination of the interatomic distances and covalent radii from such a fit was made using a computer program [8].

Recent structural studies of liquids [9] have shown that the X-ray diffraction permits determination of translational diffusion of molecules whose shape is considerably different from spherical.

References

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