Determination of the Integral Parameters of Particles

Spherical averaging of the intensity of the scattering curve caused by random orientation of particles in solution (matrix) leads to a considerable loss of information contained in the scattering data. Therefore, even if all the particles are identical and the interference effects can be neglected, usually only some integral parameters can be evaluated from the isotropic scattering curve without a priori information. Traditional methods of analyzing small-angle scattering curves from isotropic monodisperse systems will be considered in this chapter.

Basic relations for the invariants of a scattering curve are derived in Section 3.1, while Section 3.2 deals with the problem of the number and accuracy of the structural parameters that can be determined from the given scattering curve. Section 3.3 treats practical approaches to the calculation of the invariants.

One of the most widely used approaches to the interpretation of small-angle scattering data is a “trial-and-error” modeling method. The experimental scattering intensity is compared with the scattering curves of a number of model bodies chosen on the basis of a priori information on the particle. Scattering by simple geometrical bodies is considered in Section 3.4, while Section 3.5 is devoted to approximation techniques for calculating model intensity curves. Some applications of the described methods are given in Section 3.6.

3.1. Geometrical and Weight Invariants

In this section equations for the invariants of small-angle scattering curves will be obtained. The term “invariants” denotes the structural
parameters of a particle that can be directly related to the intensity curve $I(s)$.

### 3.1.1. Total Scattering Length and Radius of Gyration

First, the behavior of $I(s)$ at very low angles will be examined. To this end one can substitute the Mclaurin series

$$
\sin(sr)/sr = 1 - s^2 r^2/6 + s^4 r^4/120 - \ldots
$$

(3.1)

into equation (2.23). If we restrict ourselves to the first two terms, then in the vicinity of $s = 0$

$$
I(s) = I(0)(1 - s^2 R_g^2/3)
$$

(3.2)

where

$$
I(0) = 4\pi \int_0^D \gamma(r)r^2 dr
$$

(3.3)

and

$$
R_g^2 = \frac{1}{2} \int_0^D \gamma(r)r^4dr / \int_0^D \gamma(r)r^2 dr
$$

(3.4)

The expression on the right-hand side of equation (3.2) can be regarded as the first two terms of the Mclaurin series of function $\exp(-s^2 R_g^2/3)$. Thus, to an accuracy of terms proportional to $s^4$, one can write for the beginning of the scattering curve

$$
I(s) = I(0) \exp(-s^2 R_g^2/3)
$$

(3.5)

This is the Guinier equation, derived nearly 50 years ago (Guinier, 1939). In order to relate parameters $I(0)$ and $R_g$ to the structure of a particle, we substitute equation (3.1) into the Debye equation (2.17) and obtain

$$
I(s) = \int \int \rho(r_1) \rho(r_2) d\mathbf{r}_1 d\mathbf{r}_2 - \frac{s^2}{6} \int \int \rho(r_1) \rho(r_2) |\mathbf{r}_1 - \mathbf{r}_2|^2 d\mathbf{r}_1 d\mathbf{r}_2
$$

(3.6)

Comparison of equations (3.6) and (3.2) enables one to deduce from the leading terms on the right-hand side that

$$
I(0) = \left| \int \rho(r) d\mathbf{r} \right|^2
$$

(3.7)

This is just the square of the total particle scattering length.