Investigations of Polymer Substances

The structure of polymers is a very important field of application for small-angle X-ray and neutron scattering methods. Small-angle scattering research can be conducted both in solutions of various concentrations and in a solid (amorphous, crystalline) state. These investigations very often provide information on the structure of polymers not obtainable by other methods.

Polymer substances as a subject of study by small-angle scattering have several specific features. Thus, as a rule, the polymer macromolecules both in solution and in an amorphous state form a fairly loose conformation (the statistical coil); crystals of polymers consist of randomly oriented aggregates of lamellar layers. The polymer samples are practically always polydisperse — they contain molecules with different molecular mass. Therefore, special interpretation methods, different from those discussed in Part II, are used for analyzing the structure of polymers.

Section 6.1 deals briefly with the basic conformation models of polymer macromolecules and the patterns of small-angle scattering by these models; the influence of polydispersity of the polymer samples is analyzed. Section 6.2 demonstrates application of the models under discussion to structural analysis of polymers in solution and in an amorphous state.

Methods for investigating lamellar structures formed by polymers crystallized from solution or from a melt are described in Section 6.3. Certain types of oriented polymer objects and possibilities for analyzing their structure using anisotropic small-angle scattering are discussed in Section 6.4.
6.1. Models of Polymer Chains

In this section we discuss briefly the basic models used to describe chain macromolecules in solution and present expressions for the small-angle scattering intensity obtained by these models. We shall not elaborate on the conformation theory of chain macromolecules, which can be found in a number of monographs by, for example, Volkenshtein (1963), Morawetz (1963), and Flory (1969).

6.1.1. Gaussian Chains

The model in which the chain is visualized as a combination of $N$ linked elements (statistical segments), each $l$ long (among other things they can be represented by $N$ monomeric units each of dimension $l$) is very convenient for describing the conformation of the chain macromolecule. This schematic concept is shown in Figure 6.1. There might be two types of interaction in this chain: short range, between adjacent elements of the chain; and long range, between elements distant from each other in the chain but close in space.

Here, only the presence of short-range interactions can be assumed; whether or not there are long-range interactions is determined by the solvent containing the polymer chain and their presence leads to additional effects, that will be discussed in Section 6.1.4.

Polymer macromolecules are capable of assuming a multitude of conformations, so it is reasonable to talk only about their statistically averaged characteristics in solution. The average distance between the elements of the chain is one of the most important such characteristics. It can be demonstrated that for the $i$th and $j$th elements of the chain,