APS de Gennes Symposium New Orleans

Quasi-elastic scattering – theory and experiment hand in hand Julia S. Higgins Imperial College, London, UK

In his early career de Gennes worked with colleagues at the CEA Saclay and was familiar with the new possibilities offered for studying materials using neutron scattering techniques. Slides 2 -4 give the relevant neutron properties and the temporal and spatial scales available from the quasi-elastic scattering technique. Slide 5 shows that for polymers an unusual power law behaviour was observed compared to diffusion in simple liquids. de Gennes published a number of papers in this field, two of the most influential being in the field of polymer dynamics where he developed theoretical descriptions of quasi-elastic scattering from single polymer chains in solution. The first results were based on the Rouse model of a polymer chain with no dynamic interaction with the solvent – slide 6. The second paper (slide 7) appearing a little later extended the theory to take account of hydrodynamic interactions with the solvent (the so-called Zimm model).

These papers appeared at the time when high resolution quasi-elastic scattering techniques were being developed at a number of neutron sources and were influential in driving some of the first experimental investigations of polymer dynamics using neutrons (slides 8, 9, 10). As dynamic light scattering developed, particularly from large biological molecules the theory was also applied here. Neutron experiments were carried out by measuring energy changes in the scattered neutrons and thus for model fitting the energy spread in the incident neutron beam had to be convoluted with the chosen model – seriously inhibiting the choice of the correct model as shown in slide 10.

The subsequent development of the reptation model for polymer molecules in the dense phase (slides 11, 12, and 13), and the publication by de Gennes of the scattering law expected from a reptating chain (slides 20, 21) also coincided with developments in experimental techniques, in particular the neutron spin-echo technique (slides 14 to 18). This technique allowed the scattering from single polymer molecules in dense phases to be observed and provided some of the first direct experimental tests of the reptation model (slides 22 to 26). Quasielastic scattering and particularly neutron spin-echo techniques have been continually developing in subsequent decades, and both local side group dynamics and main chain motion have been investigated in detail, well as collective motions in these glass forming material (slides 27 to 33). Interpretation of the data has been considerably advanced by the parallel development of modelling, particularly molecular dynamic simulations. New neutron sources with even higher fluxes currently being commissioned include QENS in their portfolio of instruments (slides 34 and 35) so that we can anticipate further experimental investigation of polymer dynamics, to compare to ever more sophisticated modelling.