Quasielastic scattering – theory and experiment hand in hand

JULIA HIGGINS, Imperial College, London

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. He 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. The second paper appearing a few years 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. As dynamic light scattering developed, particularly from large biological molecules the theory was also applied here. The subsequent development of the reptation model for polymer molecules in the dense phase, and the publication by de Gennes of the scattering law expected from a reptating chain also coincided with developments in experimental techniques, in particular the neutron spin-echo technique. 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. 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, as well as collective motions in these glass forming materials. 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 so that we can anticipate further experimental investigation of polymer dynamics, to compare to ever more sophisticated modelling.