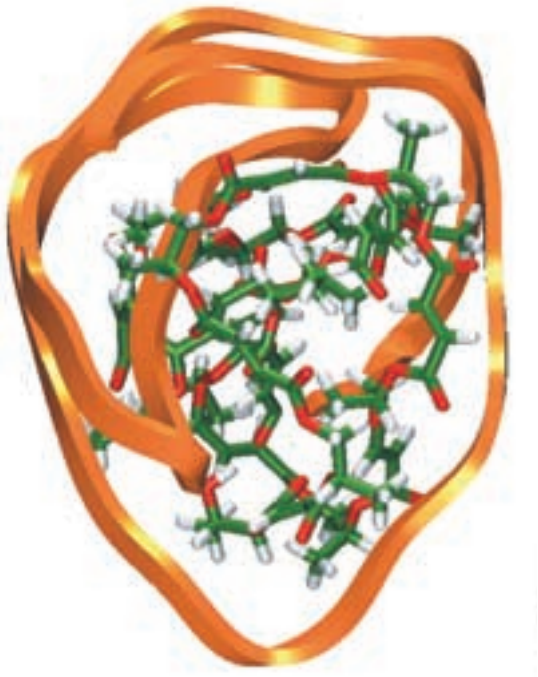
Experimental and Theoretical Investigation of Complex Polymer Structures (SUPERNET)

An ESF scientific programme



The European Science Foundation acts as a catalyst for the development of science by bringing together leading scientists and funding agencies to debate, plan and implement pan-European initiatives.

The ESF scientific programme Experimental and Theoretical Investigation of Complex Polymer Structures (SUPERNET) *addresses the current key questions in polymer science:*

- *What are the relationships between macromolecular structure, supramolecular structure, supermolecular structure and the physical properties of materials?*
- *In what way can the combination of experiments and molecular modelling help us to understand the phenomena that govern polymer behaviour?*

The programme will investigate a variety of functional polymers, copolymers, networks, branched polymers and liquid crystalline polymers in order to better understand the formation of complex topological structures.

The SUPERNET programme was established in 1999 by ESF. Member Organisations contribute to the programme over a five year period. The programme offers different types of grants to both young and senior scientists to foster exchange and joint experiments, and organises workshops and conferences relevant to the programme.

The Steering Committee guiding the programme is composed of expert scientists nominated by the ESF Member Organisations contributing to the programme.

Polymer materials today

In the search for more effective ways to create new engineering and speciality polymer materials vast activities have been undertaken and development costs spent on blending and making compatible different components in order to improve materials properties. The application of multicomponent copolymers and interpenetrating polymer networks allows the combination of different properties of incompatible polymers. Depending on reaction conditions and the choice of component monomers, polymer materials with structures in the range of nanometers to micrometers can be prepared. Such multicomponent copolymers and networks can combine the classical properties of polymers with new functionalities for novel high technology applications.

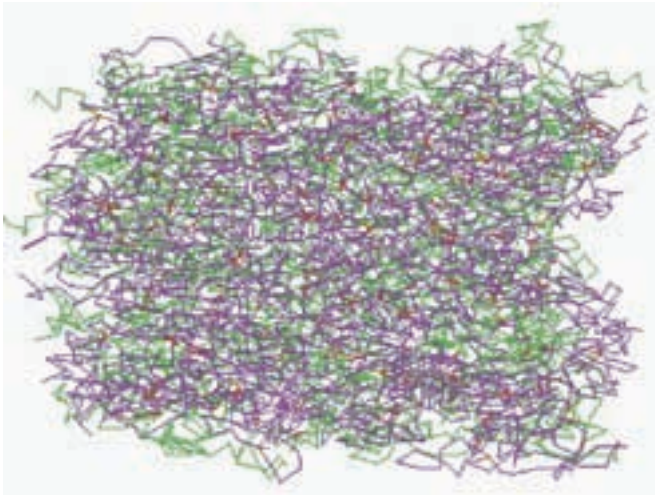
Scientific aims of SUPERNET

The aim of the project is to combine experimental and theoretical studies of block copolymers, networks, branched polymers and liquid crystalline polymers to gain a deeper understanding of two fundamental aspects of polymer science.

The first is the process of formation of complex topological structures such as branched polymers and multicomponent or interpenetrating networks and ordered polymers.

The second is the correlation between the materials properties and the chemical structure of the constituent monomers or polymer blocks.

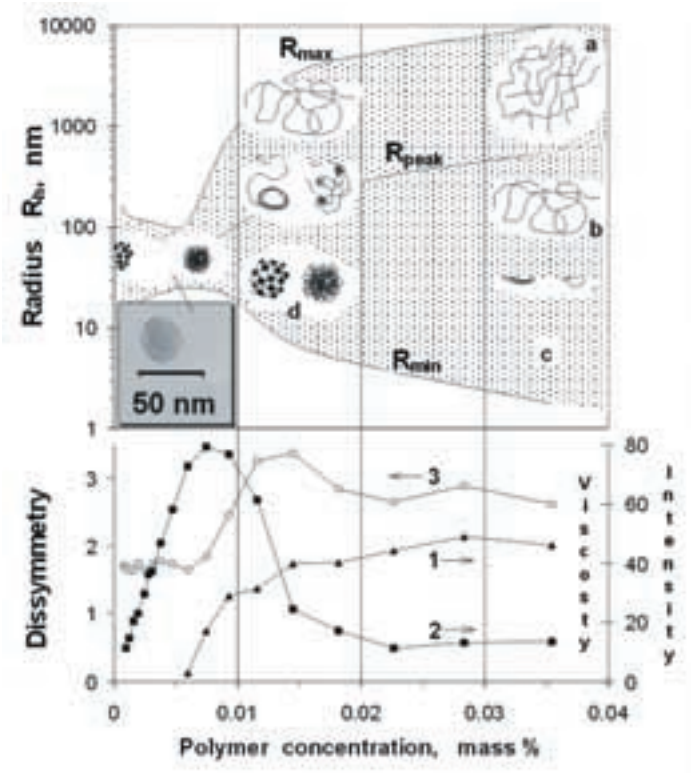
The ultimate goals of this project will be the study of the influence of polymerisation conditions on the morphology and typology of the materials, and the composition and compatibility of the components on the physical properties of the products.



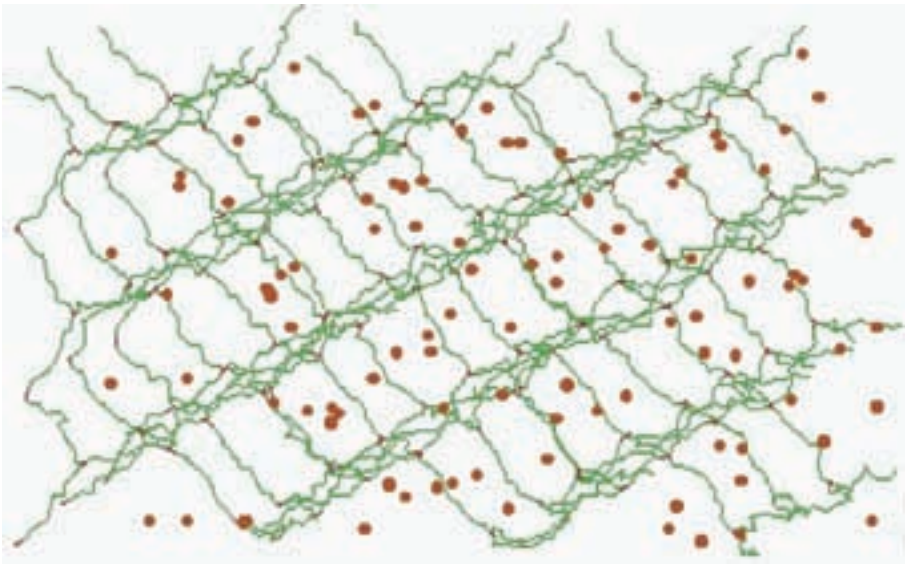
A model for simulation of two component interpenetrating networks has been elaborated. The figure shows the configuration of two interpenetrating networks with repulsive interactions between the components. Relaxations of the strands in the network occur faster than those of similar linear chains in the melt. The local inhomogeneity of the density distribution of the networks is seen in the figure.

The research project will involve methods of specific polymer synthesis and copolymer synthesis. Block copolymers consisting of blocks with different physical and chemical properties will be prepared and characterised. Copolymers which form nanostructures based on the electrostatic attraction-repulsion between the blocks will be investigated. Advanced spectroscopic, scattering and calorimetric methods will be used in the characterisation. A very important part of the project is the modelling and the development of theory. This work will involve atomistic modelling, molecular mechanics, molecular dynamics and stochastic methods to determine the conformational mobility of single chains and assemblies of chains. The theory of relaxation in polymer brushes, oriented polymers and in polymer networks will be developed. New computer codes for parallel computers will be worked out since the group has access to powerful parallel computers in the UK and in Finland.

Advanced experimental methods are available within the network for the characterisation of multicomponent polymers and networks. Wide experience of application of NMR relaxation methods, ultrasonic and dielectric relaxation methods, measurements of rheological and mechanical properties, neutron, X-ray and laser light scattering analysis form the basis of the experimental work on complex polymer structures. Atomistic molecular modelling, molecular mechanics studies and molecular dynamics simulations are accomplished. At the same time new highly efficient algorithms of computer simulation both for branched polymers and polymer networks consisting of flexible polymer chains, and for linear polymer chains with strong orientational interactions are elaborated by the participants. Dynamic theory both for polymer networks consisting of flexible chains and for linear polymer chains with strong orientational interactions is also improved within the network.



A polycation, poly(methacryloylethyl trimethylammonium methyl sulfate), with $<M_w>$ = 2.5×10^6 g mol^{-1} shows interesting solvent dependent conformational changes. A coil - globule transition has been shown to occur in mixtures of acetone and water containing a small amount of sodium hydroxide. The upper part of the scheme represents changes in the coil size distribution as a function of polymer concentration. Probable polymer conformations in solution; a) a transient network, b) single coils, c) partially globulised and, d) fully globulised polymers. Light scattering data obtained at a scattering angle of 90^0 represent average maximum and minimum values of the radius of gyration, R_h, respectively, and the highest value of distribution. The lower part of the scheme shows the concentration dependence of 1) the reduced viscosity, 2) the light scattering intensity and, 3) the angular dissymmetry parameter. The viscosity data are in dl g^{-1}, while the intensity is given in counts of photons per s, $'10^{-4}$ cps. Insert: a micrograph of a polymer globule.



Computational methods have been introduced to gain a better understanding of the molecular level processes governing the transport and distribution of small molecules in polymer networks. The incorporation of small molecules in an extended polymer network system is shown. The model allows the study of both the network and the diffusion of the small molecules inside it.

The experience of all participating groups in preparation and characterisation as well as in theoretical description of polymer systems will be combined to develop novel approaches for syntheses of multicomponent materials with new functionalities.

The greatest emphasis is on polymer systems with outstanding mechanical, electrical and optical properties as well as environmental response. Control of the influence of polymerisation conditions on the morphology and topology of the products, and also control of the influence on the composition and the phase behaviour of the polymers, will be the ultimate goal in this project. New advanced methods of polymer synthesis and analysis of molecular, supramolecular and supermolecular assemblies will be designed. Theory and simulation methods for complex polymer structures will be developed. New efficient computer codes for parallel computers will be advanced.

SUPERNET activities

Workshops and conferences

The Steering Committee organises international workshops which are held about once a year. An initial meeting with around 35 participants was held in Strasbourg, France, at the ESF headquarters on 19-21 November 1999. The next workshop will be held at the same venue on 17-19 November 2000. In addition a large international EURESCO Conference will be held in

Finland in 2001. Workshops are planned on specific aspects of the SUPERNET programme, such as specific polymer synthesis, relaxation measurements or theoretical modelling. The Steering Committee invites proposals from potential organisers, in particular in the countries participating in the SUPERNET, on topics with a clear connection to the scientific goals and the working programme of the SUPERNET programme.

Short-term fellowships

These are for young scientists, who need further training and expertise in new experimental and modelling methods for a fruitful continuation and broadening of their research scopes. Short term fellowships are intended to facilitate the transfer of knowledge and techniques relevant to research from one laboratory to another within Europe (at least one contributing country should be involved). The grants are for periods up to six months and the amount will be between 1 070 and 1 375 Euros per month plus travel expenses. Selection rounds are 15 April and 15 November each year. Applications should reach the ESF office prior to the relevant date.

Short scientific visit grants

These cover the costs of short visits of senior researchers working in the area of the SUPERNET programme, in order to carry out joint experimental or theoretical work primarily in one of the SUPERNET participating laboratories. Applications for short scientific visit grants are treated in the same way as the short-term fellowship applications, and should involve at least one contributing country.

Funding

ESF scientific programmes are principally financed by the Foundation's Member Organisations on an *à la carte* basis. SUPERNET is supported by:

Fonds voor Wetenschappelijk Onderzoek – Vlaanderen, Fonds National de la Recherche Scientifique, Belgium; Statens Naturvidenskabelige Forskningsråd, Denmark; Suomen Akatemia/ Finlands Akademi, Finland; Centre National de la Recherche Scientifique, France; Deutsche Forschungsgemeinschaft, Germany; Slovenska Znanstvena Fundacija, Slovenia; Teknikvetenskapliga Forskningsrådet, Sweden; Engineering and Physical Sciences Research Council, United Kingdom.

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For the latest information on this programme consult the SUPERNET home page: *www.esf.org/supernet*

Cover picture:
Core and shell structure of an AB diblock copolymer consisting of an unsaturated polyester block and a poly(ehylene glycol) block.The polyester chain forms the core.

November 2000

IREG Strasbourg - Dépôt légal: novembre 2000 - N° d'ordre: 002815