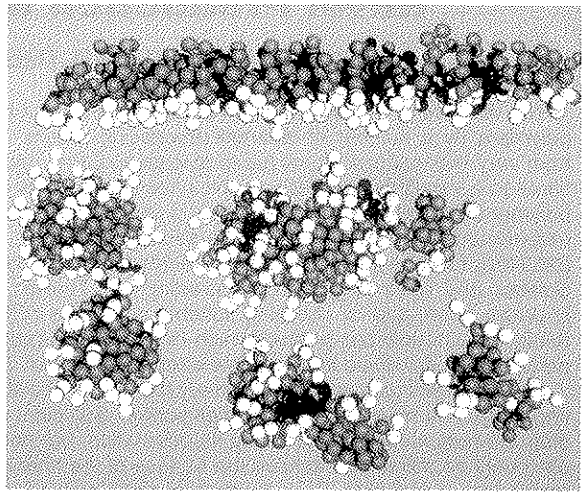
Smi927

Surfactants Can be Modelled

DYNAMICAL PROCESSES IN MICELLES REPRODUCED



Snapshot of part of the surfactant/water system. For clarity only the surfactants are shown; the white spheres are the hydrophobic segments. A monolayer has formed at the interfaces of micelles in the water phase.

Amphiphilic molecules such as surfactants, lipids, or detergents have an affinity for both water and oil. The polar head of the molecule is hydrophilic, while the hydrocarbon chain is responsible for the affinity for oil. Dissolved in water, surfactants tend to aggregate in micelles. Micelles are simple forms of self assemblies. At higher surfactant concentration, various different assemblies such as bi-layer, cylindrical micelles, vesicles, and other structures may form. Despite the importance of these assemblies in various processes — ranging from the transport of molecules through upper-cell membranes to the removal of stains in a washing machine — our knowledge of self-assembly at a molecular level is still very poor. Computer simulations may contribute to a better understanding of these fascinating systems.

In our simulations we have used a simple water surfactant/model. The starting points of the model are: oil and water do not like each other, and a surfactant is an amphiphilic molecule, *i.e.*, one side of the molecule likes oil but dislikes water, the other side likes water but dislikes oil. Both water and oil particles are modelled with a truncated Lennard-Jones potential. The truncation of the potential is made dependent on the type of interaction such that the oil-water interactions are purely repulsive and the water-water and oil-oil interactions attractive. A surfactant is made up by several oil and water particles connected *via* harmonic springs [Smit B., *et al.*, *Nature* **348** (1990) 624; *J. Phys. Chem.* **95** (1991) 6361; *Langmuir* (in press) 1992]

Computer simulations on a water/surfactant system with 32 000 particles were performed on a network of 400 transputers using a parallel molecular dynamics algorithm [Esselink, K., Smit, B., and Hilbers, P.A.J., *J. Comp. Phys.* (in press) 1992]. The simulations were started from a completely random distribution of surfactant. A snapshot of a small part of the equilibrated system is shown in the figure. It demonstrates that micelles have formed spontaneously.

One of the remarkable results of our simulations is that we can observe the dynamical processes in a micellar solution. The typical time scale of these processes have been determined experimentally. For example, the time scale for individual surfactants to leave a micelle is 10^{-8} to 10^{-6} s, the fusion of two micelles takes 10^{-5} to 10^{-4} s, and the typical lifetime of a micelle is of the order of 10^{-3} to 10^{-1} s. These time scales are clearly (far) out of the range accessible by simulations on realistic models, where the maximum simulation time is of the order of 10^{-9} s.

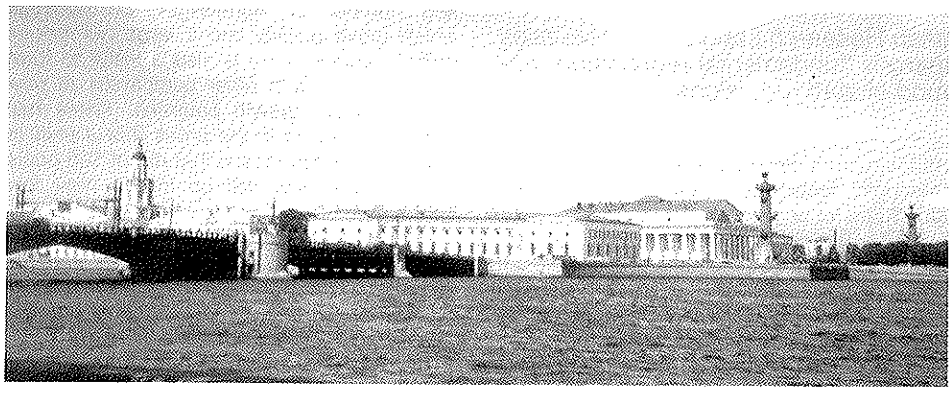
It turned out that our simple model does show these phenomena in a time span that is accessible in a computer simulation. This allows us to use molecular dynamics to study the dynamical processes that are of importance in many biological and industrial applications.

B. Smit
Shell Research, Amsterdam

Orientational Phenomena in Polymers

25th EUROPHYSICS CONFERENCE ON MACROMOLECULAR PHYSICS

St. Petersburg, Russia
6 -10 July 1992



The Winter Palace in St. Petersburg

Polymers widen the range of material properties because their molecules are large; in the case of thermoplastics. Extreme properties occur when molecules are aligned with chain connectivity along one direction. In such circumstances the familiar properties of polyethylene, for example, are much changed and it then behaves as a one-dimensional diamond, with an axial Young's modulus some 50% higher than that of steel. Such was the potential first widely appreciated a quarter of a century or so ago: it is now a reality with the increasing range of high-performance fibres and oriented polymers that are generally available in the market-place.

The Europhysics conference in St. Petersburg brought together the principal international investigators in this active field and provided a timely opportunity to review prospects and to look ahead. The chosen themes were wide-ranging, encompassing amorphous as well as crystalline systems, liquid as well as solid states, mechanisms of formation as well as resulting properties, understanding as well as knowledge. Due prominence was given to mechanical behaviour, but a notable session on conducting polymers, including a talk by P. Smith and U. Shirakawa brought much order into a particularly fast-moving area. It also emphasized that orientation improves with conductivity and mechanical behaviour in parallel, so that highly conductive systems tend to have good mechanical properties.

On mechanical aspects not only were the pioneers (Ward, Keller, Pennings, Lemstra, and others) present in person but each showed in their characteristic way the importance of current achievements and the rich potential the field still holds for the future (see box).

Scientifically, the conference was unquestionably first class, for the quality of its contributions, the discussion which was stimulated, and the personal contacts which were established and renewed. Logistically the conference was quite extraordinary. It had seemed to many that to organize any meeting in the circumstances of present-day Russia

Novel Production Methods

HOT COMPACTION OF POLYMERIC FIBRES

The last twenty years have seen the development of high stiffness and high strength polymers by a number of different processing routes. The materials produced range from very high stiffness fibres (up to at least 90 GPa), manufactured by drawing isotropic fibres to a very high draw ratio, to thick-section products produced by pressing or pulling polymer through a die, whose stiffness is usually limited to <40 GPa. There is therefore a requirement for high stiffness, thick-section materials. A process [*British Patent:* GB 2253420] for manufacturing such materials has been developed at the IRC in Polymer Science and Technology, Leeds University, UK. Termed "hot compaction", it takes highly drawn fibres and by choosing suitable conditions of temperature and pressure produces a homogeneous product which retains a high proportion of the original fibre properties while achieving a reasonable strength [*J. Mater. Sci.*, to be published].

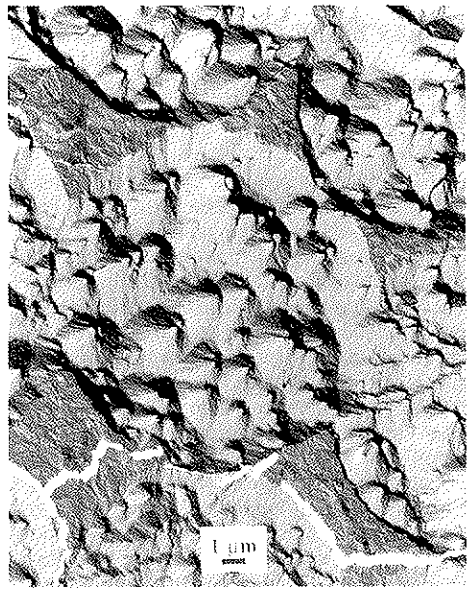
The important step was the discovery that it was possible to take a fibre below its melting range and selectively melt a small portion. Sufficient pressure needs to be applied to stop the fibre shrinking and losing its orientation, but not enough to inhibit melting. It is obviously an advantage to have the surface of the fibre melt first and anything that promotes this is desirable. For a hexagonal close-packed structure (a unidirectional arrangement of fibres) only 9% of the second phase is needed to fill all the holes and bind the structure, allowing substantial retention of fibre properties.

On cooling, the molten material recrystallises to form a second, lower melting point phase, clearly evident in differential scanning calorimetry. Morphological studies show the second phase to form a transcrystalline bridge between the fibres. The spaces between the fibres are completely filled with the melted and recrystallised polyethylene. Compaction is seen to be complete, and the fibres are in the main, still largely circular in cross-section.

Nucleation of the second phase is all along the fibre boundaries so that crystals grow out perpendicular to the fibres, meeting in the middle and forming a very strong bond. There is evidence from fracture studies that failure of the compacted composite occurs within the fibre itself, suggesting the melted and recrystallised material forms an excellent "glue", and that the weakness is within the fibre itself. This is confirmed by compaction studies on a range of fibres, which show the most highly aligned fibres (*i.e.*, those with the lowest transverse properties) as having the lowest composite transverse strengths.

Fibres so far successfully compacted include melt spun, melt kneaded and gel-spun polyethylenes, polypropylene and PET. Other fibre configurations can be compacted including chopped fibres, woven fibre cloth and laminates of unidirectional fibres. All of these have improved strength compared to unidirectionally aligned fibres, but have lower stiffness. The compacted composites allow a light, tough and high stiffness composite to be manufactured using a single phase. This has considerable advantages over processing two-component composites.

P.J. Hine and I.M. Ward, *IRC in Polymer Science & Technology, Leeds, UK*
R.H. Olley and D.C. Bassett, *University of Reading, UK*



A photomicrograph, perpendicular to the main fibre direction, of an etched cross-sectio through hot-compacted polyethylene fibre.

would not be possible: but not to Professor V. Marikhin, Dr. L. Myasnikova and their colleagues. They accomplished the impossible and organized a Conference which was exceptional in every way. To attend and live in St. Petersburg in the season of the white nights was a great privilege for the twenty five western scientists who joined ninety Russian colleagues at this most pleasant and scientifically valuable occasion. The only cautionary note is that, in contrast to previous experience, very few attended from countries of the former eastern bloc: obtaining hard currency is the new barrier to attendance. This will need to be addressed to ensure that in future good science and scientists from all countries are able to attend Europhysics conferences. The next meeting is titled "Transitions in Oligomer and Polymer Systems" (Ulm, Germany; 27 September – 1 October 1993).

D.C. Bas
Chairman, EPS Macromolecular Board

IBM RESEARCH

Shifting Emphasis to Remain Vital

Dr. Karl Kümmerle, Director of the IBM Zurich Research Laboratory, discusses the impact on basic research of the company's "fundamental redefinition" announced last November, and the latest round of staff reductions.

IBM's Zurich Research Laboratory with a staff of about 200 represents a fairly small part of the Research Division (3300 staff and an annual budget of 600 M$US which has remained almost constant for several years). It is dwarfed by IBM as a whole (300 000 employees; 69 000 M$US turn-over in 1991). Founded in 1956, established on the present site in 1962, expanded in the 1970's, modernised and expanded again in the mid-1980's, the Zurich lab, with its two Nobel prizes for discovering scanning tunnelling microscopy and high-temperature superconductivity, has acquired an outstanding reputation in basic physics research. Principal interests in physics and laser science are novel microscopies to the nanometre scale, high-Tc superconductors, numerically intensive computation, nanostructure electronic devices, novel spectroscopic techniques, and materials and structures for semiconductor lasers.

IBM's Research Division was organized formally in the 1960's to seek and exploit scientific discoveries. The 1970's saw increased emphasis on transferring technology to development and manufacturing units via joint research. There evolved some 20 programmes exploiting 30-35% of research resources. The most recent shift in strategy aims to encourage competitiveness using a less monolithic approach. There are now nine relatively autonomous business units, each of which contributes an assessed amount for corporate research and can access research capabilities. As even a company the size of IBM can only handle a limited number of "lightweight" partnerships which move quickly into a large number of niche markets, there is also a trend to form joint ventures with other companies to provide sufficient growth potential. There has been speculation in the press that a shift to applied research means that about 100 posts in basic research will go in the next few years.

***Editor** – One of IBM's goals was to be "famous for our science". Is this still the case? James McGroddy, your Director of Research, speaks of this science being a "vital" part of IBM. What does he mean ?*

Dr. Kümmerle – IBM has dual goals: it wants to be famous in science and technology and its science must also be relevant, in other words vital to IBM. The situation was established a long time ago and it is "burned in": it's part of the culture. We are famous by putting down stakes in selected field opposed to a "me too" strategy. The dual goal remains durable and nothing has changed in this respect.

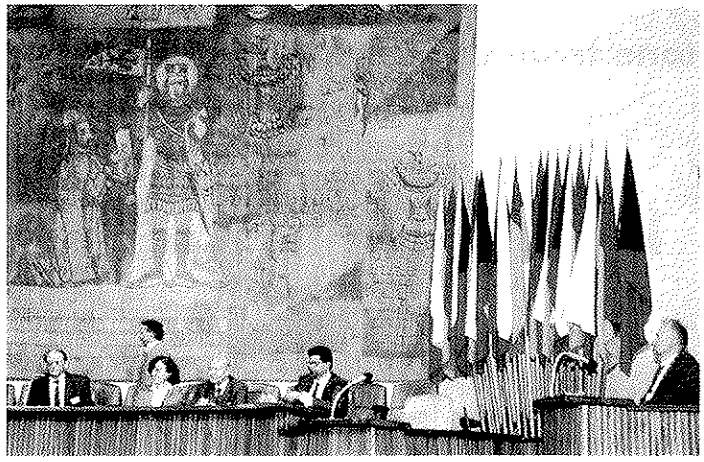
CP '92

'nternational Conference on Computational Physics

24-28 August 1992,
Prague, Czechoslovakia

CP '92 formed one in the series of conferences organized by the Computational Physics Interdivisional Group of the EPS and the Computational Physics Division of the American Physical Society, with the even years in Europe and the odd years in the USA. The first meeting took place in Boston in 1989; the second in Amsterdam in 1990; the third in San Jose last year, while next year's conference will be organized in Albuquerque, USA. Some 195 people from 24 different countries registered for CP '92. Monday, the 24th was devoted to tutorials on the processing of scientific documents, features of Fortran, neural networks, parallel algorithm design, cellular automata, visualization, symbolic computing, and networking a physics department. The Plenary sessions were held on the Tuesday. A fair part was in the form of two-minute introductions to posters, where it was remarkable how some speakers managed to interest the audience in their poster in such a short time. Wednesday and Thursday offered sessions and posters in parallel; there were only plenary sessions on the closing day.

Being a conference organized by an interdivisional group, the range of subjects was naturally quite broad. Session topics included (quan- um) molecular dynamics, physics education, dynamical systems, electronic structure, fluids and plasmas, mesoscopic physics, Monte Carlo simulations of quantum systems, new trends in hardware and software, Monte Carlo techniques, self-organization and coherent structures, symbolic computing, nano computing, and non-equilibrium phase transitions and critical phenomena.



The CP'92 opening ceremony in the magnificient Aula Maxima of the University of Prague's Carolinum.

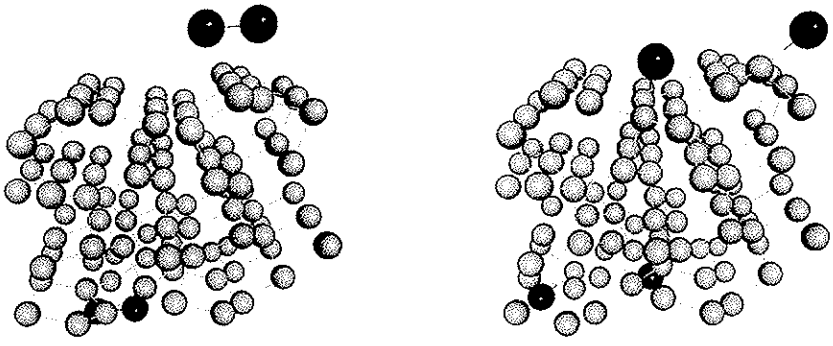
Some highlights of the conference are described by the authors themselves in accompanying boxes. The main trend of the conference was clearly dominated by the impact of massively parallel machines, both now, but especially in the rather near future, and how Europe can play a rôle in this.

The APS-EPS Steering Committee on Computational Physics met and endorsed the plan to organize the 1994 meeting in Manno (near Lugano), Switzerland.

R.A. de Groot, *Chairman, CPG*

First Application of a New Approach

FIRST-PRINCIPLES PARALLEL SIMULATION OF MOLECULAR DISSOCIATION



First-principles simulation of chlorine dissociation on the silicon (111) surface. Left and right panels show snapshots of the system as the molecule first approaches the surface, and 0.15 picoseconds later, with chlorine and silicon atoms shown as large and small spheres, respectively.

The last few years have seen a revolution in the computer simulation of condensed matter. Previously, simulations were based on simple models for the interactions between atoms. Increasing computer power is now making it possible to perform fully realistic simulations of matter based on first-principles quantum mechanics.

A collaboration between research groups at Cambridge and Keele Universities in the UK reported to the Prague CP '92 conference on the first application of first-principles simulation to study molecular dissociation at a solid surface [Stich, I., Payne, M.C., De Vita, A., and Gillan M.J., CP '92 Poster: *First-principles dynamics used to study dissociative chemisorption*]. Apart from the new science presented, the work was also technically novel in that the simulations were performed on a massively parallel supercomputer — a 64-node Meiko Computing Surface at Edinburgh University. This is the first time that parallel processing has been used for the first-principles simulation of dynamical processes.

The way molecules dissociate when they strike the surface of a solid is important for understanding many different processes, including surface catalysis, corrosion and the operation of gas sensors. There has been a vast amount of experimental work, but many questions remain unanswered. Does the molecule dissociate as it sticks to the surface, or does it stick first and dissociate later? How does the dissociation process depend on the energy and angle of incidence? How do the answers to these questions depend on the molecule and the surface material? First-principles simulation offers for the first time a way of reproducing and analysing what happens when a molecule hits a surface under specified conditions.

The Cambridge-Keele poster presented preliminary results of first-principles simulations of a chlorine molecule striking the (111) surface of silicon. The methods used build on ideas originally proposed in a seminal paper by R. Car and M. Parrinello [*Phys. Rev. Lett.*, **55** (1985) 2471]. For each set of atomic positions as the system evolves in time, Schrödinger's equation for all the valence electrons is solved to determine the electronic ground state. The interaction of these electrons with each atomic core is represented by a "pseudopotential", with electron correlation treated by the local density approximation (LDA). This allows the forces on all the atoms and hence the full time evolution to be calculated. The experience of many research group has demonstrated the accuracy and reliability of pseudopotential-LDA methods.

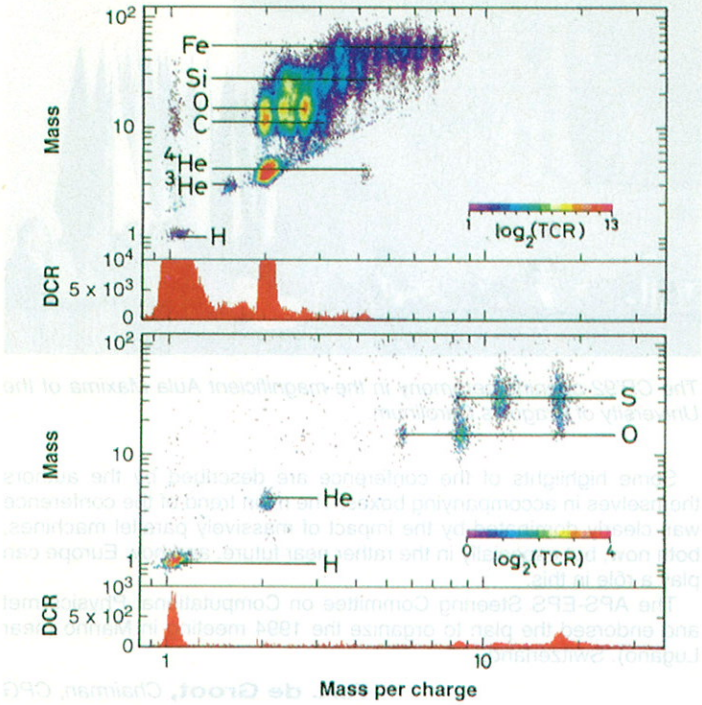
A number of dynamical simulations were reported, with the chlorine molecule started in different orientations a short distance outside the surface, and projected towards different sites on the surface. The figure illustrates what happens when the molecular axis is initially parallel to the surface. Dissociation occurs spontaneously and very rapidly, and at the same time both chlorine atoms form new chemical bonds with the surface atoms. The indications are that this may be a general feature at the fairly high incident energy of 1 eV used in the present simulations.

The authors stress that the work is still in progress, but what seems clear is that first-principles dynamics opens a new way of attacking some unsolved problems concerning molecular processes at surfaces.

M.J. Gillan
Keele University, UK

JOVIAN ATMOSPHERE

Ions from the Satellite Io Dominate



The mass versus mass/charge matrices of the solar wind well after the encounter (upper) and of the Jupiter magnetosphere (lower). The triple coincidence rates (TCR) are colour coded in the upper parts of the panels while the double coincidence rates (DCR), for which mass information is unavailable, are given in histograms below.
The two ion populations differ in two important respects: elemental abundances and charge states, the former owing to the dominating contribution of Io material in the Jovian magnetosphere (there are larger amounts of S and O ions). The q/M data indicates that solar wind ions are nearly equilibrated in the ≈10^7 K environment of the low corona.

The Solar Wind Ion Composition Spectrometer (SWICS) aboard Ulysses allows the determination of the mass loading of the rotating magnetic field of Jupiter, which in turn determines the effect of centrifugal forces on the geometry and dynamics of the Jovian atmosphere. SWICS combines energy-per-charge separation by an electrostatic analyser (0.6 to 60 keV/*e*), acceleration (23 kV), time-of-flight (tof) measurement, and determination of total energy with solid-state detectors. For an ion producing a triple coincidence (two tof and one solid-state detector signals), this technique allows the determination of ion mass *M* and charge *q* separately so that different ion species can be distinguished even if they have equal *M*/*q* ratios. A double coincidence (tof only) permits only measurement of *M*/*q*. The coincidence methods used suppress background, an important feature in the strong radiation fields of the Jovian magnetosphere.

SWICS measured for the first time the composition of the main plasma in the magnetosphere at very different distances from Jupiter and at different latitudes. We found everywhere a strong contribution of ions for Io, and that some solar wind ions penetrated deep into the magnetosphere. We were even able to identify unambiguously ions from Jupiter's atmosphere far away from the planet.

Io is an exceptional body in our Solar System. It is similar in size to the Moon and thus, like the Moon, too small to produce (4.5 Gy after its formation) an endogenous volcanism. Io's strong volcanism bringing relatively volatile material (including O and S) to the surface results instead from a kneading caused by Jupiter's tidal forces. This material overcomes the gravitational attraction of Io, probably with the help of electromagnetic forces, and escapes into the magnetosphere and eventually leaves Jupiter's sphere of influence. Io ions dominate the mass density of the Jovian atmosphere and cause the ion composition to be exceptional.

Previous spacecraft had found that much of the Jovian atmosphere was rich in O and S ions from Io. The new findings extended measurements to other regions, thus placing more severe constraints on models of plasma circulation, radial transport, and loss from the magnetosphere, with the identification of ion masses needed for proper assessment of terms in mass-balance equations.

The SWIC's experiment involves groups from Bern University, TU Braunschweig, MPI für Aeronomie, University of Maryland (USA), and NASA's Goddard Flight Center. European participation in all Ulysses experiments is conceived, managed and implemented by institutes and universities with national funding.

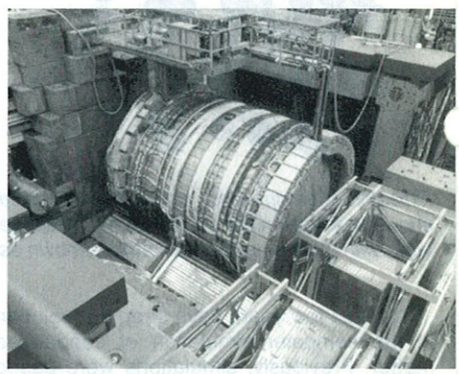
J. Geiss, *Bern University*

HERA Enters Second Phase of Data Taking

DESY in Hamburg collided electron and proton bunches for the first time a year ago in its new HERA storage ring complex. Machine studies then concentrated on the lifetime of the proton beam and the first examination of the transverse polarization of the electrons. There followed a nearly four-month shutdown to move the two large experiments H1 and ZEUS into position. A major concern of high-energy ep colliders, of which HERA is the first and probably the only one for many years to come, is that the proton beam would be sensitive to excitations caused by the opposing electron beam because it does not experience synchrotron radiation damping. These effects turned out to be sufficiently weak, provided the beam sizes at the interaction point are well-match and the proton betatron tuning is optimised.

So the run-up to the 820 GeV proton design energy was tackled with confidence starting in April; protons were stored at this energy for the first time in May 1992. The electron energy has been kept slightly below the 30 GeV design value to continue earlier work on polarization and stability. Data taking with collisions of single electron and proton bunches first occurred on May 31 and continuous experimental operation began about a month later. Operation until early in August gave 20% availability to experiments using 10 stored bunches in both rings, but with 20% of the design level for the proton bunch intensity pending more work on the proton pre-accelerators. A drastic reduction of the electron beam's lifetime at higher beam currents was observed on attempting to increase the luminosity by increasing the numbers of electron and proton bunches. The origin of this effect is not yet fully understood. The luminosity for the 10-bunch mode normalised to the beam intensity has reached the design value so in this crucial respect, HERA performs to expectations.

A second phase of data taking started in September and runs until November. The machine's availability is already rising and peak luminosity is expected to be increased by increasing the number of bunches. Wulfrim Bartel of DESY says the first physics results mainly address three topics. The total cross-section for photon production has been measured in a hitherto unexplored energy range (230 GeV in the centre of mass). It is rising, but not as steeply as some models predict. Regarding the structure of the photon: strong indications for so-called resolved photon processes reflecting quark structure have been observed for the first time. Thirdly, for deep inelastic scattering, HERA studies the structure of the proton at high momentum transfers (Q^2) and at values of *x*, the proportion of the momentum of the proton carried by the quark, some 10^2 times smaller than for previous experiments. H1 and ZEUS have also looked for exoti particles like leptoquarks and excited electrons, but for this type of research more data is clearly required.



HERA's H1 detector being moved into position. Both H1 and Zeus, the other HERA detector, are now being used routinely.