

Computational Physics in Industry

B. Smit

Shell Research and Technology Centre, Amsterdam

In an industrial context one rarely has the possibility to select the simplest systems for molecular simulations. Aims are set by business objectives rather than scientific convenience, and the imposed boundary conditions may require special attention. Increasing computer power may of course allow one in some cases to apply well-established and reliable fundamental methods to more complex systems. For some problems, however, the increase in computer time is prohibitively large so novel algorithms must be developed. It will be shown that a new Monte Carlo technique allows the simulation of systems of industrial interest that were considered impossible to study by molecular techniques. This development is illustrated by two examples: the adsorption of alkanes in zeolites and the phase behaviour of long-chain alkanes.

Adsorption in Zeolites

Zeolites are crystalline inorganic polymers that have a well-defined microporous structure. These pores are accessible to various guest molecules. The large internal surface, the thermal stability and the presence of acid sites make zeolites an important class of catalytic materials for petrochemical applications.

Catalytic conversion inside the pores can be seen schematically as involving the absorption and diffusion of the reactants, catalytic conversion, and diffusion and desorption of products from the zeolite. The overall activity and selectivity of a particular reaction is the result of a delicate balance of these three processes. Much experimental and theoretical effort aims to understand each of the steps at a molecular level. The high selectivity of zeolites implies that the behaviour of the adsorbed molecules is system-specific. It is therefore essential to be able to study the behaviour of the adsorbed molecules of interest under reaction conditions. Unfortunately, this is very difficult, particularly for long-chain hydrocarbon molecules.

Computer simulations, used with molecular dynamics or Monte Carlo techniques, are an attractive alternative to experiments because they can, in principle, provide information for conditions under which experiments are not feasible.

However, simulations have been limited to atoms or small molecular guest molecules and could not be extended to molecules of catalytic relevance. For example, the diffusion of the straight-chain alkanes butane and hexane from one channel to another in the zeolite silicalite is very slow and the rate of diffusion decreases with increasing chain length. Unacceptably long simulations are therefore required to obtain reliable results.

The Monte Carlo technique is not limited by the slow diffusion of molecules because diffusion barriers are by-passed by making moves to arbitrary positions in the zeolite. For chain molecules, however, this is not the case because the probability of finding a position without overlap between hydrocarbon and zeolite decreases exponentially with chain length. To be able to use Monte Carlo in this relatively complex system of industrial relevance it is necessary to develop novel algorithms which are orders of magnitude more efficient.

Adsorption

Consider adsorption of alkanes in zeolite. Fluids confined in narrow pores can have properties that are distinctly different from those of bulk fluids. Most studies have focused on simple fluids which can be modelled as near-spherical molecules. But molecular shape can also exert an influence on the fluid's behaviour, particularly for large, complex molecules.

Adsorption isotherms are of fundamental interest in studying fluids in pores because they may signal phase transitions, such as capillary condensation or wetting, of the fluid. For example, if a system exhibits capillary condensation, one would measure a stepped adsorption isotherm with hysteresis. As the pores of most zeolites are of molecular dimensions, adsorbed alkane molecules behave like a one-dimensional fluid. In a one-dimensional system phase transitions do not generally occur so one would expect Type I adsorption isotherms for alkanes, that is, they do not show kinks or steps. If steps occur, they are usually attributed to capillary condensation in the exterior secondary pore system formed by the space between different crystals.

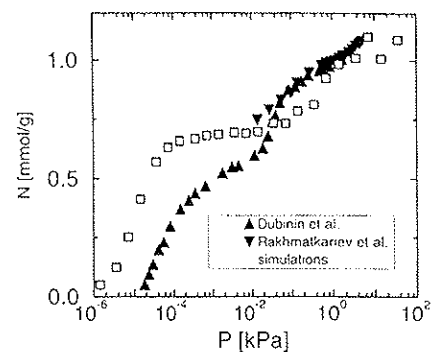


Fig. 1. Adsorption isotherms of heptane in silicalite. Closed symbols, experimental data; open symbols, results of simulations for a temperature $T = 298$ K. The number of moles of gas N adsorbed per gram of silicalite is plotted as a function of the gas pressure P .

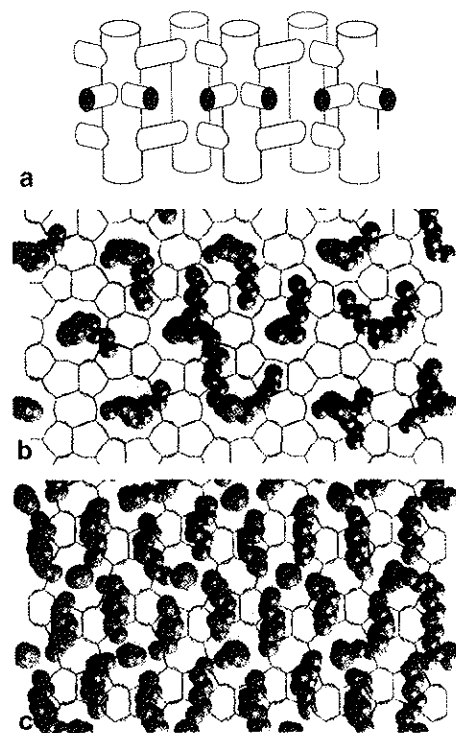


Fig. 2. Adsorption of alkanes in zeolite. A schematic illustration (a) of the pore structure of silicalite showing the wider straight channels and the narrow zig-zag channels. CBMC simulation of hexane in silicalite: b) approximately half the maximum loading; c) almost maximum loading. The zig-zag channels are in the plane of the page; straight channels are perpendicular to the page. Grey spheres represent hexane molecules; red/orange lines represent the zeolite framework.

Adsorption isotherms have been determined for various n -alkanes in zeolite silicalite. They are indeed of Type I for the short-chain alkanes (methane and pentane). For hexane and heptane, however, a kink or step is observed suggesting that some kind of phase transition takes place, but no molecular explanation has been given. At present, data on sorption properties are scarce because experiments

are difficult and time-consuming, especially under reaction conditions. Computer simulations seem to be an alternative to quantify the sorption behaviour.

A Monte Carlo Simulation

Molecular simulations of adsorption are conveniently performed in a grand-canonical ensemble, which corresponds closely to the experimental arrangement: a zeolite in open contact with a reservoir that fixes the temperature and chemical potential. The number of particles in the zeolite is allowed to fluctuate via Monte Carlo moves in which one attempts to add or remove a particle. Particularly for chain molecules, the insertion of molecules tends not to be favoured in a conventional grand-canonical simulation. To see this, consider a simulation of methane molecules adsorbed in a zeolite. Assume that a methane molecule can be inserted successfully if this molecule is placed at a randomly selected position where it does not overlap with one of the other atoms of the system. Depending on the loading, one needs on the order of 10 attempts to find such a position; for ethane this is of the order of 10, and for heptane as large as 10^{21} . The latter would result in a simulation of many years even for a super-computer, and allowing simulations to equilibrate would be prohibitively time-consuming.

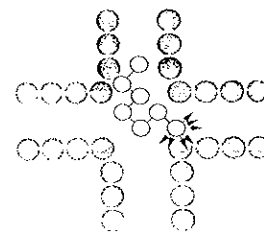
For this reason simulations of adsorption have focused on systems containing small molecules. To make grand-canonical simulations of long-chain alkanes possible, one can use the configurational-bias Monte Carlo (CBMC) technique (see insert) for the insertion step. Simulated adsorption isotherms of various alkanes in silicalite obtained using CBMC and a unified atom model (see insert) have been compared with experimental data [4]. For butane a Type I isotherm is observed, and the agreement between experiments and simulation is good. For hexane and heptane, there is reasonable agreement at high pressures, but at low pressures deviations exist which indicate that the zeolite-alkane model can be further improved.

More importantly, for heptane both the experiments and the simulations show a step at approximately half the loading (Fig. 1). Detailed inspection of the calculated adsorption isotherm shows a kink at this loading for hexane. As the simulations are performed on a perfect single crystal, these deviations from the Type I isotherm must be due to a transition of the fluid inside the pores and cannot be attributed to the secondary pore system.

Configurational-bias Monte Carlo

In configurational-bias Monte Carlo [1] a molecule is not inserted at random but is inserted atom-by-atom in such a way that overlaps are avoided. This "growing" procedure introduces a bias which leads to an incorrect distribution of configurations. This bias can be removed exactly [2] by using the weight introduced by Rosenbluth and Rosenbluth [3] to correct the biasing of acceptance of trial conformations and not the thermal averages as was originally proposed. The probability of generating a particular conformation is then proportional to the conformation's Boltzmann weight, thus removing the main drawback of the original Rosenbluth scheme.

A simulation is performed in cycles, and each cycle consists of a number of randomly selected moves: displacement of particles, rotation of particles, partial regrowing of a molecule, and regrowing of a molecule at a randomly selected position. The figure illustrates the growing of an alkane in a zeolite in a CBMC move. The black circles represent the atoms of the zeolite, and the white circles the atoms of the alkane. Seven atoms have



been grown successfully, and an attempt is made to insert the eighth. The arrows indicate seven trial positions for which the energy u_i is calculated. One is selected with a probability given by $p_i = \exp(-u_i/k_B T) / w_{\text{new}}(l)$ where $w_{\text{new}}(l) = \sum_j \exp(-u_j/k_B T)$ for a temperature T and Boltzmann constant k_B . Similarly, for the old configuration, one calculates $w_{\text{old}}(l) = \sum_j \exp(-u_j/k_B T)$. This is repeated until the entire chain of length m has been grown. The bias of the growing is removed by the replacement of $\exp(-\Delta U/k_B T)$ by $\prod_{l=1}^m w_{\text{new}}(l) / \prod_{l=1}^m w_{\text{old}}(l)$ in the acceptance rule. This Monte Carlo technique can be 10 to 50 orders of magnitude more efficient than molecular dynamics (the number of trial orientations in the CBMC moves for the adsorption simulations ranged from five for butane to eight for heptane).

United-Atom Model

In a united-atom model for alkane molecules the CH_3 and CH_2 groups are considered as single interaction centres, with pseudo-atoms in a given chain connected by rigid bonds. Non-bonded interactions are described by truncated Lennard-Jones potentials; intramolecular interactions include bond-bending and torsion. The zeolite is modelled as a rigid crystal and alkane-zeolite interactions are

assumed to be dominated by dispersive interaction with oxygen atoms which are described by a Lennard-Jones potential. Size and energy parameters are fitted to the heats of adsorption and the Henry coefficients of n -alkanes in silicalite. Simulations of the absorption isotherms used periodic boundary conditions for a box contained 16 unit cells of silicalite with total size $40.14 \times 39.840 \times 53.680 \text{ \AA}^3$.

Silicalite has two types of channels, straight and zig-zag, which are connected via intersections (Fig. 2a). Figs. 2b and c shows "snapshots" of hexane molecules in the channels of silicalite at two different loadings: Fig. 2b is at approximately half the maximum loading and in Fig. 2c the zeolite is almost saturated. Note that the length of a hexane molecule is of the order of the length of the period of the zig-zag channel. At low chemical potential, the hexane molecules move "freely" in these channels and the molecules will be in the intersections for some of the time. If part of the intersection is occupied, other molecules cannot reside in the straight channels at the same time.

At high pressures, almost all the hexane molecules fit exactly into the zig-zag channel (Fig. 2c): they no longer move freely and keep their noses and tails out of the intersection. In such a configuration the entire straight channel can be tightly packed with hexane molecules. This explains the plateau in the adsorption isotherm: in order to fill the entire zeolite

structure neatly, the hexane molecules located in zig-zag channels have first to be frozen in these channels. This freezing of the positions of the hexane molecules in the channels implies a loss of entropy, so an increased pressure or chemical potential is needed. This increase is reflected as a step in the adsorption isotherm.

The incommensurate freezing of n -alkanes which just fit into the zig-zag channels has been confirmed recently using temperature programmed desorption [5]. In contrast to other alkanes, both heptane and hexane show a second desorption peak at low temperatures corresponding to desorption of the low entropy molecules found in the zig-zag channels at high loadings.

Traditionally, research on the applications of zeolites in the petrochemical industry has focused on trying to understand catalytic conversion in the pores of the zeolite; less attention has been paid to the sorption properties *per se*. This lack of knowledge has long hampered the understanding of phenomena such as the

"compensation effect" – an unexpectedly high conversion of long-chain alkanes seen in catalytic cracking which has only recently been attributed to differences in the sorption behaviour of the alkanes. The example described above shows that quantifying sorption using computational techniques such as configurational-bias Monte Carlo is not only a prerequisite for the design and optimization of catalysts, but also leads to a better understanding of the fundamentals of zeolite catalysis.

Phase Equilibria

Alkanes are thermally unstable above approximately 650K, which makes experimental determination of the critical point of alkanes longer than decane extremely difficult. The longer alkanes, however, are present in mixtures of practical importance for the petrochemical industry. The number of components can be so large that it is impractical to determine all phase diagrams experimentally. One has therefore to rely on predictions made by equations of state where the parameters are directly related to the critical properties of the pure components. Data are scarce and contradictory, so semi-empirical methods are used to estimate the critical properties.

Configurational-bias Monte Carlo has been combined with the Gibbs-ensemble technique (see insert) to simulate the vapour-liquid equilibria of the *n*-alkanes at conditions where experiments are not (yet) feasible.

Most models for the vapour-liquid equilibrium of alkanes have been obtained by fitting simulation data to experimental properties of the liquid at standard conditions. Since the phase diagrams are very sensitive to the choice of interaction potentials, models can be improved by fitting predicted critical properties to experi-

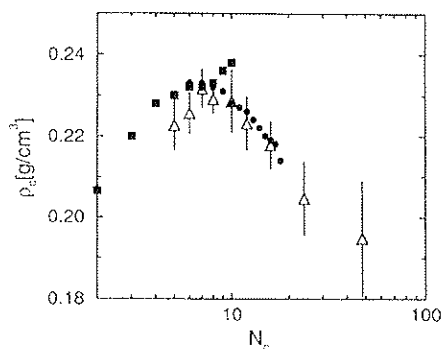


Fig. 3. The critical density of *n*-alkanes as a function of the carbon number N_c . The open symbols for the simulation data show a maximum at $N_c \approx 8$ and the closed symbols are for two sets of experimental data, one of which shows a plateau at $N_c = 8$.

CBMC and the Gibbs Ensemble

The Gibbs-ensemble scheme was introduced [6] as an efficient tool to simulate vapour-liquid phase equilibria, where the simulations of the phases are carried out in parallel. Monte Carlo rules which allow for changes in the number of particles and the volume ensure that the two boxes representing the two phases are in thermodynamic equilibrium with each other. Since the two boxes are not in "physical contact", there is no interface and the bulk properties of the two coexisting phases can be obtained directly with a surprisingly small number of particles.

This makes the Gibbs ensemble extremely

Beyond Chain Molecules

CBMC is not simply a method for generating conformations of chain molecules since it is much more general. It can be used as a scheme to perform collective rearrangements of any set of labelled coordinates. In fact, the scheme can be used to carry out Monte Carlo moves to swap *n* small particles within a volume ΔV with one large particle that occupies the same (excluded) volume. This application has been exploited to study mixtures of large and small hard spheres [T. Biben, unpub.]. Gibbs-ensemble simulations of mixtures of spherical colloids and rod-like polymers have been performed [9] using CBMC-style particle swaps and a closely related approach was used to study phase separation in mixtures of hard-core particles on a lattice [10]. Applying CBMC to improve the sampling of ionic solutions has been proposed [11].

A different application of the CBMC ideas involves an algorithm to perform Monte Carlo moves in parallel has been developed by Esselink *et al.* [12]. Parallel Monte Carlo appears to be a contradiction in terms, since the Monte Carlo procedure is an intrinsically sequential

process: one has to know whether the current move is accepted or rejected before continuing with the next move. The conventional way of introducing parallelism is to distribute the energy calculation over various processors, or to farm out the calculation by performing separate simulations over the processors.

Although the latter is extremely efficient and requires minimum skills, it is not a truly parallel algorithm. For example, farming out a calculation is not very efficient if the equilibration of the system takes a significant amount of processor time. In the algorithm of Esselink *et al.* several trial positions are generated in parallel and the one with the highest probability of being accepted is selected with the highest probability. This selection step introduces a bias which is removed by adjusting the acceptance rules. The generation of each trial move, which includes the calculation of the energy (the Rosenbluth factor in the case of chain molecules), is distributed over the various processors. The approach has been used to calculate phase equilibrium in parallel using the Gibbs-ensemble technique [13].

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References

- mental data. This results in simulations which reproduce critical temperatures fairly well [7]. However, this is not the case for the critical density, largely because there is considerable disagreement between the experimental data.
- Much of the current knowledge on the critical properties of the higher alkanes is based on extrapolating experimental data, usually as a monotonically increasing function of the carbon number. CBMC simulations predict a maximum critical density at about C_8 (Fig. 3). Some experimental data give a plateau at C_8 while other show no evidence of a maximum. It is interesting to note that Monte Carlo simulations of the vapour-liquid curve of a polymeric bead-spring model for various chain lengths [8] show a decrease of the critical density as a function of chain length. This phenomenon is a general feature of long-chain molecules, as has already been pointed out by Flory.

A Premier Event

G. Chiarotti who chaired the International Programme Committee of the 15th General Conference of the Condensed Matter Division of EPS (Baveno-Stresa; 22-25 April 1996), reports that the conference has established itself as one of the premier events in its field.

To point out the highlights of a conference is always a difficult task. Doubtless one makes more enemies than friends! Nevertheless I shall try to summarise my general impressions of 15th General Conference of the Condensed Matter Division of EPS which took place beside Lake Maggiore last April. The remarks are biased of course by my own scientific interests and tastes.

Some of the more exciting results discussed at the conference dealt with Bose-Einstein condensation in (extremely) cold alkali vapours, a phenomenon that was discovered only a few months ago. In a plenary invited talk, W. Ketterle, who works on the team that made the first observation in sodium at MIT, described the fantastic cocktail of experimental techniques (extremely low temperatures, laser imaging, etc.) that led to the observation of a condensate of as many as 5×10^3 atoms [see EN 27 (1996) 105]. The conference was also able to offer an invited talk on the theory of Bose-Einstein condensation in

magnetically trapped atomic gases by S. Stringari, and an contribution by P. Wachter on the excitonic insulator in rare-earth compounds, a system that is believed to undergo Bose-Einstein condensation.

Computational physics, especially molecular dynamics and Car-Parrinello *ab-initio* simulations, was a subject that undoubtedly received great attention. Once limited to special problems in solid and liquid dynamics, it has now pervaded almost every field of condensed matter. Computational results were presented for matter under extreme conditions, especially high pressures; diffusion; soft matter; etc. The conference offered a total of eight invited talks and eight oral contributions on computational physics. They were complemented by a plenary lecture by E. Tosatti on order-disorder transitions at surfaces, which although based primarily on physical concepts and intuition often relied on *ab initio* calculations. Another plenary talk in the special session on

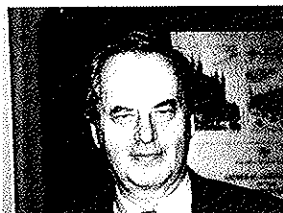
applied physics – by B. Smit on the catalytic cracking of oil molecules (see page 189) – also spoke in detail about the results of simulations. Some of the problems are indeed formidable so physical intuition (fortunately!) still plays a crucial role. Paradigmatic in this respect was the title *Physical Chemistry with Computers and Intuitions* of the invited talk by M.L. Klein.

The session *Semiconductors and Insulators* was by far the largest as it covered several related symposia and more than 250 submitted contributions. A great deal of research in this field is devoted to nanostructured materials (including quantum wells, wires and dots, clusters and fullerenes, carbon nanotubes and microactivities, etc.). An interesting trend, clearly noticeable at the conference, was that these techniques, once limited to semiconductors, are now spreading to other fields such as superconductors (antidot lattices; artificial multilayers for high- T_c superconductivity), magnetic materials, assisted diffusion, etc., where nanoscale fabrication opens up unexpected possibilities. A plenary invited talk *New Phenomena in Nanostructured Materials* by Y. Bruynseraede surveyed applications in superconductors and metals.

Reduction of length scales allows the observation of quantum interference effects and their use in electronic devices. We are all well acquainted with band-gap engineering in semiconductors. F. Capasso in his plenary lecture showed that wavefunction engineering is also possible through the control of layer thickness in multilayer structures. Taking advantage of the structure of the wavefunction, it is now possible to control the transition probability of electrons across the barriers, increasing or suppressing emission at certain energies. Through such mechanisms, quantum cascade lasers that emit as much as 100 mW in the infrared (5-10 μm) have been built.

A result of fundamental research, and one that can be traced to the same type of problem, is the observation of coherent dynamics of a single-electron wavepacket in KBr using femtosecond laser techniques. The authors (R. Scholz *et al.*; contributed paper) were able to follow the time evolution of the wave packet of the excited electron in the F-center, observing damped periodic oscillations of the sample transmission in the THz range. The configurational coordinate model (once inferred from the Stokes shifts in luminescence) can now be checked directly by observing the vibronic frequencies.

Speakers at the CMD'96 Special Plenary Session on Applied Physics that was chaired by G. Chiarotti, the Chairman of the CMD'96 International Programme Committee. From the left, F. Capasso (AT&T Bell Laboratories, NY, USA), B. Smit (Shell Research, Amsterdam) and O.V. Lounesmaa (Helsinki).



Industrial exhibitors are an important feature of all major conferences that seek to promote the application of physics research. Some 25 companies exhibited at CMD'96, among them Magnetic Solutions, Ltd. a start-up founded in 1994 by academic and research staff from Trinity College, Dublin (TCD). The company, which is based at the TCD Innovation Centre, designs and manufactures advanced magnet systems, some of which are sold under the slogan "Forget Electromagnets". To understand why, please read the article on page 186 by J.M.D. Coey, the company's Managing Director, who spoke during the CMD'96 symposium. He is photographed here with David Hurley, the company's Manager, on the left. The Centre aims to start up 2-3 new companies each year in areas in which the university can contribute and become involved; they then usually move out after about three years.

Magnetic Solutions is unusual in that it has started manufacturing within a comparatively short time. One innovative product is a compact pneumatically driven permanent magnet flux source based on an original system of split-pair Halbach cylinder permanent magnets (page 188). The source shown in the photograph generates large, switchable magnetic fields which are ideal for synchrotron beamline experiments.

MAGNETIC SOLUTIONS



Another result that depends in a dramatic way on improvements in experimental techniques was presented by F. Sette in a plenary lecture. The availability at the European Synchrotron Radiation Facility in Grenoble of intense and collimated beams of X-rays allowed him to reach energy resolutions of 3.2 meV with beams of 10-20 keV. As an example, he discussed experimental results on the dispersion of longitudinal acoustic excitations in water, in a range of momentum transfer that corresponds to propagation velocities twice the speed of sound in the hydrodynamic limit [see *EN* 26 (1995) 78].

One last improvement in experimental techniques that is worth mentioning is the possibility – achieved recently using X-rays from synchrotron radiation sources – of surface-structure determinations. Such methods, which were discussed in an invited talk by R.L. Johnson on semiconductor surfaces studied with STM and x-ray diffraction, successfully complement other surface-sensitive techniques.



Stimulating employment opportunities for young physicists has become a major preoccupation. One approach is the setting up of some form of "job market" at large general conferences which have a bias towards applications. It has been very successful in the United States, where the American Physical Society's March meeting provides students and young physicists with detailed information about job openings. Offering this service has the additional advantage that young people are encouraged to attend major scientific meetings.

The same approach is poorly developed in the much less homogeneous European context. So the CMD'96 organizers made a determined effort to provide job information and counselling. This was a success and they were able to establish job placement as an integral feature of the CMD conference series (CMD'97 takes place in Leuven on 25 - 28 July 1997). Initiatives were based on a Placement Centre where young people registered their details and received announcements from



potential employers. The Centre also hosted a series of well-attended presentations by laboratory directors and government officials, including Marco Malacarne from the European Commission's science directorate who is seen here answering questions on fellowship opportunities within European Union programmes. Another feature was an introduction to the Sportello Giovani on-line interactive WWW database of candidates seeking employment and job opportunities. The service is clearly a pioneer in using the Web to provide job information. Hosted in Genoa by the Istituto Nazionale per la Fisica della Materia (INFN) with support from the EC as an accompanying measure, it is administered by Matilde Bolla (seen on the right in the photograph with Manuela Arata, the INFN's Director General). Sportello Giovani (<http://www.infm.it>) currently details 200 job offers (80% in Europe) based essentially on published advertisements and information from Italian research agencies (INFN, INFN, CNR) and universities.

15th General Conference of the Condensed Matter Division

More than 800 scientists from 37 countries attended the 15th General Conference of the EPS Condensed Matter Division. Though the commendable efforts of the Organizing Committee and the support of some national and international agencies, a large participation (more than 100 scientists) from east and central Europe was possible. Participants from outside Europe amounted to 29.

The conference clearly established itself as a premier venue for the worldwide exchange of scientific and results in the field of condensed matter, in a way comparable to the American Physical Society's March meeting.

The conference consisted of six main sessions (Semiconductors and Insulators, Magnetism and Metals, Superconductivity, Liquids and Statistical Mechanics, Polymers and Soft Matter, Surfaces and Interfaces) and 14 symposia dealing with some of the leading fields of present research. The symposia elucidate the scientific trends covered by the conference as planned by the International Programme Committee so it is useful to recall their titles:

- High-pressure phases of low-Z elements
- Isotopically engineered materials
- Computational physics in condensed matter
- Clusters and fullerenes
- Point-contact spectroscopy
- Scanning tunnelling microscopy
- High-Tc superconductors
- Vortices in superconductors and superfluids
- Magnetic nanostructures
- Observation of surfaces at atomic resolution
- Atomic mobility and tunnelling
- Semiconductor nanostructures and cavities
- Conducting polymers
- Thin polymer layers and interfaces.

The conference offered a relatively large number of plenary invited talks (12, including the lecture by R.H. Friend, the winner of the 1996 Hewlett-Packard Europhysics Prize) and invited talks (69 in parallel sessions). Some 180 contributions papers were presented orally and 660 as posters.

The Programme Committee aimed to stress the importance of condensed matter research in the development of our society by organizing two special events. The first was a full morning plenary session devoted to applied solid-state physics with invited talks by J.M.D. Coey on *Industrial applications of permanent magnets*, F. Capasso on *Quantum cascade lasers*, E. Smit on *Computational physics in industry*, O.V. Lounasmaa on *Medical applications of SQUIDS in neuro- and cardiomagnetism*, and R.H. Friend on *Semiconductors device physics with conjugated polymers*. There was also an evening plenary session devoted to Science and Society with an invited talk *Past, present and future of industrial research in solid-state physics* by J.C. Phillips [see *EN* 27 (1996) 125] followed by an impromptu discussion, coordinated by N. Kroó, on European Union programmes.

A forum on (proposed) new European large facilities (far-infrared free-electron lasers, physics in the megagauss region, and cold neutron sources) with three invited speakers (K. Unterrainer, M. Springford, A. Furrer, respectively) was organized as a special parallel session.

Other plenary invited lectures were by: R.A. Cowley on *Are there two lengths scales at a phase transition?*; W. Ketterle on *Observation of Bose-Einstein condensation in ultra-*

A. Stella, the Conference Chairman, on the left, with G. Chiarotti.



cold atomic gases; E. Tossatti on *Order and disorder at crystal surfaces*; T.P. Martin on *C₆₀ molecules with a metallic outer layer*; F. Sette on *Collective dynamics in liquid water by inelastic X-ray scattering with meV resolution*; Y. Bruynseraede on *New phenomena in nanostructured materials*.

Mention should be made of the Placement Centre (see above) and twelve "young author awards" for the best contributions presented by young scientists (under 30 years of age) were offered by the Istituto Nazionale per la Fisica della Materia.

The conference was a great success. Attendance at the sessions (including the closing session) was very high and the discussions were always lively and extended. And the weather remained acceptable for most of the time! Moreover, the participation of young scientists exceeded expectations. The people who made this success possible were A. Stella (Conference Chairman), I.C. Andreani (Scientific Secretary), G. Guizzetti (Chairman of the Local Committee), and the members of the International Programme Committee, namely V.M. Agranovich, M. Altarelli, F.J. Balta-Calleja, F. Bassani, R. Cantelli, M. Cardona, G. Chiarotti (chair), F. Cyrot-Lackman, J.T. Devreese, J.E. Enderby, E. Flores, P. Fulde, V.V. Mishchalkov, R.J. Nocholes, M. Parrinello, E. Rimini, M.P. Tosi, P. Wachter, K. Wandelt, and P. Wyder.