Meetings

Computer Experiments

The 1971 Battelle Colloquium on Interatomic Potentials and Simulation of Lattice Defects was held in Seattle, Washington, and Harrison Hot Springs, British Columbia, from 14 to 19 June 1971 (*1*). It was the first large-scale meeting ever held on methods, techniques, and results of computer experiments. The proceedings of the meeting (*2*) will be dedicated to George Vineyard, who led the group which developed the first computer experiment system at Brookhaven National Laboratory during the period 1957–60. The following excerpts from Dr. Vineyard's introductory lecture define the topical content of the meeting and outline its scope.

> High-speed computers have made possible an interesting class of investigations. Starting with an atomic model of a crystal lattice or liquid, the behavior of the model is directly computed to elucidate physical phenomena. Complex models with many degrees of freedom, displaying phenomena resistant to analytical treatment and to definitive study by experimental means, have been employed, and the results have been surprising and enlightening. The picturesque term "computer experiments" is appropriate for such work. In a sense this is a third estate of physics.
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> In the relatively short time that computer experiments with lattice models have been under way, a remarkable range of work has been done. Looking over these results one could conclude . . . that a golden age is dawning. . . . In many potential areas of computer experimentation, the pioneering work has hardly been done, let alone the careful follow-ups needed for maturation of the field.
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> Above all, better interatomic potentials are needed. The various computer experiments that are done with lattices require an enormous range of interatomic energies from the fractional eV [electron volt] interaction at normal lattice spacings to the hundreds of kilovolt interactions called into play in radiation damage cascades and ion bombardments.

Five introductory lectures were given during a 1-day session at the Battelle Science Center in Seattle, Washington. The session started with a review, "Computer experiments with lattice models," by Vineyard, followed by A. A. Maradudin on "Lattice dynamical defect problems" and W. A. Harrison on "Interatomic potentials in solids." A lecture by N. W. Ashcroft concerned "Ion-ion interactions in metals" and one by N. H. March dealt with "Displaced charges in relaxed defect lattices."

The colloquium then moved to Harrison Hot Springs for the presentation (in 1-day sessions) of research papers devoted to interatomic potentials, point defects, dislocations and stacking faults, and surfaces and interfaces. In each session, the existing experimental evidence was reviewed in addition to results of theoretical and computer-experiment work. Each research paper was followed by a discussion, and each session was amplified by an agenda discussion held during the evening. In addition, there were an agenda discussion on computer-experiment techniques and a concluding agenda discussion on critical issues, the latter session directed by A. Seeger.

Reports on the construction of interatomic potentials from first principles were given by N. W. Ashcroft, L. A. Girifalco, W. A. Harrison, and M. P. Tosi. The construction of empirical potentials was covered in papers presented by R. Chang, J. M. Cowley, J. E. Enderby, R. A. Johnson, N. H. March, M. T. Robinson, and W. D. Wilson. Results of computer experiments on the properties of point defects were given by J. R. Beeler, R. Bullough, D. G. Doran, P. S. Ho, R. A. Johnson, L. B. Pedersen, I. M. Torrens, and W. D. Wilson, and the properties of dislocations and stacking faults were covered in papers given by M. S. Duesberry, P. C. Gehlen, J. R. Parson, R. Perrin, W. R. Tyson, and V. Vitek. Surfaces and interfaces were treated by R. E. Dahl, G. Ehrlich, D. P. Jackson, M. F. Kanninen, M. J. Weins, F. W. de Wette, and P. Wynblatt. Computer experiments on quantum phenomena were described by J. H. Weiner, and A. Rahman described some of his new results on liquid-state computer experiments, including recent work on water. J. R. Beeler, L. A. Girifalco, J. P. Hirth, A. Seeger, and P. G. Shewmon served as agenda discussion leaders.

To explain the achievements of the colloquium in the appropriate technical perspective, it is necessary to outline the typical computer-experiment approach employed in an attempt to characterize the behavior of a defect in a crystalline lattice.

Most computer experiments on defects in crystals are carried through, in practice, by dividing the discrete crystallite into two regions: (i) a central region, containing the defect core, in which the displacements of atoms from their perfect crystal positions are large, and (ii) an enveloping mantle about the central region in which the displacements of atoms from their perfect crystal positions are small. In the central region, atoms are displaced in accordance with forces derived from a pairwise-interaction potential energy function. In the mantle, atomic displacements are defined in terms of elasticity theory for the particular defect under consideration. The elastic constants used in the mantle are those derived from the interatomic potential used in the central region. The interatomic potential is usually anharmonic, which makes it possible to account for nonlinear and anisotropic effects in the central region. In the past, isotropic, linear elasticity theory usually was adopted for computing atomic displacements in the mantle region. Hence, feedback of an anisotropic, nonlinear response from the mantle to the central region, sometimes vitally important, was usually missing. The ideal way to describe the interaction between atoms in the central region and mantle atoms would be through a Green's function technique. In practice, approximations to this ideal procedure have been employed.

The central problems encountered in computer experiments pursued in terms of this conceptual framework are (i) construction of an appropriate pairwise interatomic potential function, (ii) solution of the elasticity problem for the correct atomic displacements in the mantle region, and (iii) design of a correct computer-experiment technique for generating the large atomic displacements that occur in the central core region of the defect.

The first computer experiments on defect properties were calculations of configuration, formation, and migration

energies for point defects. The potential functions used were short-range, central-force potentials. Linear, isotropic elasticity theory was used to describe atomic displacements in the mantle.

Currently of interest are the properties of dislocations, stacking faults, grain boundaries, and free surfaces, the interactions between these extended defects, and their interactions with point defects. In the discussions of dislocations, stacking faults, and grain boundaries, the participants in the colloquium indicated a need for noncentral, medium-range potentials and nonlinear, anisotropic elasticity theory. In addition, they indicated that point-defect calculations should be repeated with noncentral potentials. In this respect, a new generation of point-defect calculations has been started by R. A. Johnson and W. D. Wilson. They have constructed noncentral potentials for the transition metals and have performed computer experiments on properties of point defects with these new potentials. A systematic Green's function approach has been developed by R. Bullough and V. K. Tewary. Seeger's group has begun work on computing boundary conditions in terms of nonlinear elasticity theory.

The quest for a generally valid pairwise interatomic potential is the quest for a succinct and general description of atomic interactions in crystals. No one really expects that this quest will be realized, of course. But, practically speaking, reasonably good approximations can be found for a particular problem. Apparently, this will be done by means of empirical potentials or force constants. Most of the potentials used so far have been empirical potentials in the sense that even though their functional form has been suggested by theory, they have been calibrated by fitting to experimental data. All potentials used are pertinent to a particular qualitative range of defect-property simulations, determined by the nature of the experimental data used to calibrate them. Generally applicable potentials do not exist.

Interatomic potentials specifically constructed to simulate the properties of point defects in bulk crystals have been used fruitfully in the simulation of internal surfaces such as grain boundaries. However, because of the local disruption in the electron density at a free surface, a vast amount of work remains to be done in developing suitable potentials for use in computer experiments on the behavior of free surfaces and the interactions of other defects with free surfaces. Correlations between bulk and surface properties, such as the correlation between compressibility and surface tension outlined by N. H. March, would be valuable in an empirical approach to constructing interatomic potentials for studies of free surfaces.

Three types of computer-experiment techniques are likely to dominate future work. These are the dynamical, Monte Carlo, and lattice statics methods. The dynamical method is the touchstone of computer-experiment methods. It generates the phase space for a classical system of atoms as a function of time. In principle, it can completely describe the implications of any classical physical model of an assembly of atoms. The Monte Carlo method, in essence, develops atomic configuration states in accordance with statistical mechanical laws for thermal equilibrium. The lattice statics method determines the atomic displacements associated with a crystal defect on the basis of the harmonic approximation for the energy density of a crystal.

The general problems mentioned, namely, construction of potential functions, solutions for atomic displacements in the mantle, and the design of correct and efficient computer-experiment techniques, are difficult problems. Immense amounts of hard work lie ahead in the computer-experiment field, but the impression left by the discussions was an impression of optimism.

P. C. GEHLEN
J. R. BEELER, JR.
R. I. JAFFEE
Battelle Columbus Laboratories, Columbus, Ohio 43201

Reference and Note

1. Annually, Battelle has organized a Materials Science Colloquium since 1966. The topic of the 1972 meeting is Deformation and Fracture of High Polymers, and it will be held from 11 to 16 September in Kronberg, Germany. The meetings are by invitation only.
2. P. C. Gehlen, J. R. Beeler, Jr., R. I. Jaffee, Eds., *Interatomic Potentials and Simulation of Lattice Defects* (Plenum, New York, in press).

Disease Transmission by Arthropods

At least 80 percent of all infectious disease is arthropod-borne and yet minimum research effort has been directed toward an understanding of the dynamic roles of the arthropod vector and host in disease transmission. The vector's capacity for disease transmission and the host's response to the vector are determinants which have been studied primarily on a unidisciplinary basis, that is, without collaboration by specialists in different fields. There has been little attempt at a multidisciplinary examination of the factors that determine the outcome of the interaction between host, vector, and parasite. Such an opportunity was made possible through a symposium held in Hamilton, Montana, on 15 September 1971, sponsored by the Tropical Medicine and Parasitology Study Section, Division of Research Grants, National Institutes of Health, and by the Rocky Mountain Laboratory, National Institute of Allergy and Infectious Diseases, NIH. Members of the laboratory and of the study section and other interested specialists met to consider current knowledge on the interactions of arthropod vectors with hosts and infectious agents, and to identify areas requiring further investigation.

Reviews of current knowledge were presented in two main topic areas: (i) intra- and interspecific variations in the capability of vectors to transmit disease agents, and (ii) the host response to arthropod bites. Vector-to-host transmission of the causative entities of arbovirus disease, hemorrhagic, spotted and tick fevers, plague, tularemia, malaria, filariasis, and tick paralysis were discussed. Tick paralysis, an ascending motor paralysis induced by tick salivary gland toxin, is an example of a disease considered in the first topic area. Female ticks from each of 14 generations of *Dermacentor andersoni* raised at the Rocky Mountain Laboratory failed to induce paralysis, whereas the opposite was true of ticks from each of 11 generations of the same species derived from a field site where frequency of paralysis was high. Such intraspecific variation in ability to cause or transmit disease, suggestive of single gene dominance, has been observed also in mosquito vectors of malaria and filariae. With arboviruses little is known beyond the laboratory observation that vector capability is related to the amount of virus ingested by the vector.

In the second topic area there is little information on intraspecific variability in the response of hosts to