atomic parameters makes any human participation in the calculations very tedious. If solving protein structures were as important as reaching the moon, this problem could be solved rather quickly. However, with such a small fraction of most national resources devoted to basic research, it seems likely from this conference that the crystallographers in the world may have to continue exercising their programming ingenuity on undersized computers for some time to come.

II. PHASE TRANSITIONS

By ***Gabrielle Donnay***

Of the forty papers contributed at the symposium on phase transitions, nine unfortunately came after the deadline and thus will not appear in the printed abstracts. The symposium was divided into eleven sessions, three of which were devoted to invited one-hour lectures.

The first of the invited papers, presented by M. J. Buerger of the Massachusetts Institute of Technology, preceded the symposium. Its purpose was to survey the advances made in the field and perhaps to intrigue members of the Congress into staying the first three days of the following week to learn more about the subject. I believe Professor Buerger succeeded on both counts. He showed how his structural classification of transitions into reconstructive and displacive ones overlaps the thermodynamic division into first and higher orders, and he suggested that mixed transitions may occur that involve both types of orders.

R. A. Young of the Georgia Institute of Technology spoke of his own detailed study of the mechanism of the quartz transition at 573° C, which entailed, among other things, refined structure determinations at eight temperatures below and above the transition (R indices less than 4%).

A. R. Ubbelohde of Imperial College, London, pointed out the need for just such careful single-crystal observations during phase transitions. He discussed the phenomena to be looked for, among them coexistence of multiple domains of slightly different structures, on the one hand, and continuous slight changes of one-crystal structure that remains homogeneous throughout, on the other.

These three lectures provided the stimulation that comes from hearing about an interesting subject from experts with different backgrounds and different ways of looking at the same phenomena. Thus, even without contributed papers, the symposium would have been a success.

As it was, many of the contributions illustrated the points raised by the invited speakers; others brought out new ones. The Russians are very active in this field and had eight interesting papers. Among them were the following: a new classification of magnetoelectric properties (seven in all), NMR studies of ferroelectric phase transitions, and a study of ferroelectric-antiferromagnetic transitions that accompany *compositional* changes in solid-solution series. This latter type of phase transition, which is of particular interest to mineralogists, has attracted little attention so far in this country.

The attendance at all sessions was surprisingly good, considering that even the most enthusiastic crystallographer must have been close to saturation by then. The general appreciation of this symposium is evidenced by present plans to hold another symposium on the same topic *before* the next IUCr Congress in Moscow in 1966.

III. *some aspects of* LATTICE DYNAMICS

By ***David R. Chipman***

Because of the proximity of the International Conference on Lattice Dynamics in Copenhagen from August 5 to 9,* Symposium III of the Rome meeting in September was designed, not as an opportunity for presentation of the latest results in the field of lattice dynamics, but rather as an elementary course to give the average crystallographer an understanding of the types of problems which

* See *Physics Today*, February 1963, p. 102.

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have been solved and those being studied now, the techniques which have been used and those showing the greatest promise at present. The speakers could hardly have been better chosen for this task, and there was, as a result, general agreement on the great success of the symposium.

In the introductory lecture on Monday morning, W. Cochran, organizer of the symposium, gave us a little of the history of the subject, an elementary account of the theory, and a summary of the several techniques which have been used for measurements of thermal vibrations. In the second lecture, B. E. Warren showed how dispersion curves for elastic waves can be obtained from the intensity of thermal scattering of x rays. He then described the use of lattice theory to obtain from the dispersion curves a set of interatomic force constants from which the frequency distribution of the crystal may be obtained.

B. N. Brockhouse, in discussing the role of neutron inelastic-scattering measurements in determining the thermal motion of a crystal, pointed out that the great advantage of neutron measurements is that both the energy and momentum changes of the neutron caused by the scattering can be measured, giving directly the dispersion curves. He then showed experimental dispersion curves obtained with neutrons and discussed the different models of interatomic forces needed to explain the results.

In the afternoon, J. P. Mathieu discussed the optical aspects of lattice vibrations. He described the diffusion of visible and ultraviolet light by elastic waves, the absorption of infrared radiation, and the determination of optical constants from these measurements.

W. Ludwig ended the symposium on a theoretical note, reviewing the many difficulties encountered in calculating the lattice dynamics of a crystal so essential to an understanding of thermal motions. He concluded by discussing the very current problem of handling anharmonic terms in the equations of motion and the effects of anharmonicity on measureable properties of the crystal.

AUTOMATION

a session of the Commission on Crystallographic Apparatus

By ***S. C. Abrahams***

For most crystallographers, the twin problems of how to measure integrated intensities accurately and how to measure them quickly are of daily concern. An open session of the IUCr Commission on Crystallographic Apparatus, called specifically to discuss these problems, provided a high point of the Sixth Congress. This session contained six invited papers, followed by a vigorous informal discussion held with less rigid attention to time than most other sessions.

U. W. Arndt of the Medical Research Council, Cambridge, gave a comprehensive review of basic designs in automatic analog and digital single-crystal diffractometers. S. C. Abrahams, of Bell Telephone Laboratories, Murray Hill, N. J., drew attention to many important sources of error in diffractometer measurement. Criteria were given for their detection with typical examples based on one fully automatic diffractometer. L. E. Alexander of the Mellon Institute, Pittsburgh, discussed the different experimental geometries used in making integrated intensity measurements, with particular reference to the spectral composition of the diffracted beam.

Turning specifically to neutron diffractometry, H. A. Levy of the Oak Ridge National Laboratory compared existing automatic systems and then gave an impressive demonstration of the reliability and accuracy of the new ORNL diffractometer.

Descriptions of the four automatic single-crystal diffractometers in Japan were given by S. Hoshino of Tokyo University. G. Gaglioki of C. C. R. Euratom, Ispra, then discussed some of the problems in measuring the integrated intensity of diffracted neutron beams.

An 18-minute film entitled "Automated X-Ray Diffractometry"* opened the lively informal discussion. It was generally regarded as unfortunate that the basic session on important new apparatus was scheduled to conflict with simultaneous sessions on proteins and on crystal morphology in the morning, and on six other topics in the afternoon.

* Prints of this movie are available, on request, from S. C. Abrahams, Bell Telephone Laboratories, Murray Hill, N.J.