05. X–1 COMPUTER SIMULATION OF PHASE TRANSITIONS (CRYSTALLIZATION, SOLUTION ETC.). By H. Bradaczek, Inst. f. Kristallographie, Freie Universität Berlin. W-Germany.

Starting with the well known equation for the energy of a field $E \sim \int F^2 dv$ an anisotropic field has been defined for each of the components (atoms, atomgroups, molecules) of an ensemble. By superposing the fields of the individual components the field of the ensemble can be calculated. The total energy can also be obtained by use of the convolution algorithm. Movements of the components are controlled by random values of the x,y-shifts and rotations. Only those movements are executed which lead to the preselected energy (temperature) value. Besides the field and the energy of the ensemble other parameters such as the energy of the individual components and their "cooling down time" can be preselected. The nature of the field depends on the binding character of the components. Details of the field can be provided either analytically or by providing discrete values. Presently only two dimensional processes are considered, but the procedure does not restrict to expansion to a third dimension. "Crystals" up to 500 components have been processed. By appropriate choice of input parameters different experimental conditions can be simulated. A movie film shows "online" the computation process, which is displayed on the graphic terminal. The simulation of different phase transitions coupled with crystal distortion and defects are demonstrated.
The application of the method to the simulation of chemical binding is discussed.

05. X–2
HIGHER ORDER COMMENSURATE LOCK-IN IN FERROELECTRICS. G. André, D. Durand, F. Dénoyer (Laboratoire de Physique des Solides, Bât. 510, Université Paris-Sud, 91405 Orsay, France), R. Currat, C. Vettier (ILL, 156X Centre de Tri, 38042 Grenoble Cédex, France).

Thiourea is a molecular ferroelectric compound which exhibits both incommensurate and long-period commensurate (or lock-in) phases, characterized by a polarization wave of wave-vector $q_\delta = \delta \vec{b}^*$. Neutron diffraction experiments, at ambiant pressure, have established the existence of a commensurate phase corresponding to $\delta = 1/9$ stable over a 2 K temperature interval (A.H. Moudden, F. Dénoyer, M. Lambert, W. Fitzgerald (1979) Solid State Comm., 32, 933), between the incommensurate ($0.115<\delta<0.141$) and ferroelectric ($\delta=0$) phases. Two other commensurate phases with $\delta=1/7$ and $\delta=1/3$ have been observed under hydrostatic pressure (F. Dénoyer, A.H. Moudden, R. Currat, C. Vettier, A. Bellamy and M. Lambert 1982, Phys. Rev. B 25, 1697) and later a $\delta=1/8$ electric-field-induced commensurate phase has been discovered (K. Gesi, M. Izumi (1982) J. Phys. Soc. Jpn 50, 1047 and A.H. Moudden, E.C. Svensson, G. Shirane (1982) Phys. Rev. Lett. 49, 557. A simple Landau-type argument, taking account of the space group symmetry of the paraelectric phase and of the transformation properties of the modulated order parameter, confirms that 7b and 9b superstructures are expected to be more stable than 8b ones, in perfect agreement with the diffraction results. The same type of argument indicates that a $\delta=1/8$ commensurate lock-in phase can be induced by an applied electric field.

05. X–3 TAILORING OF COMPOSITE SENSORS. By R. E. Newnham, Materials Research Laboratory, Pennsylvania State University, University Park, Pennsylvania 16802, U.S.A.

Widespread interest in robots and other remote control devices has spurred interest in sensors of all types: thermal, electric field, magnetic field, chemical, mechanical stress, and radiation. The sensitivity of these devices can sometimes be enhanced by mating two or more materials together in various connection patterns which optimize the tensor components involving the material "figure of merit". Symmetry, connectivity, percolation, and scaling effects are four of the underlying factors governing the properties of composite sensors. Examples from materials science and the biological world will be described.

05. X–4 TWIN DOMAINS AND TWIN BOUNDARIES. By Th. Hahn, Institut für Kristallographie der RWTH, 5100 Aachen, FRG.

A twin is a regular oriented intergrowth of two of more (congruent or enantiomorphic) individuals of the same crystal species. It is characterized by the twin law (twin element) and the contact surface between two twin partners (domain boundary). In most cases the domain interfaces are low-energy boundaries with good structural fit.

Transformation twins usually lead to many small domains. The important phenomenon of domain switching occurs in ferroelectric, ferromagnetic, and ferroelastic crystals (ferroic transitions). Mechanical twinning due to stress includes ferroelasticity. Of particular interest for mineralogists are growth twins, which still present many problems with respect to nucleation and growth of the twin partners. A special case is twinning by merohedry (parallel-lattice twins) or by pseudo-merohedry, where the lattices of the tw n partners have (almost) the same orientation, and the reciprocal lattices (almost) coincide. The number of possible 'orientation states' of the twin domains is the subgroup index i of the crystal point group in its holohedry, i=2,4 or 8. If a translation is suppressed in the subgroup, different 'translation states' lead to antiphase domains.

The domain structures and the domain boundaries of twins can be elucidated by several methods: X-ray topography, light and electron microscopy, optical activity, pyroelectricity, piezoelectricity. The atomic structure of the domain boundaries, however, presents problems. Here model building is used, taking into account the bulk structure, the twin element, the orientation of the twin boundary and the criterion of 'low-energy boundaries'. Examples of domain structures and models of domain boundaries will be given, with emphasis on minerals and related compounds, both from the literature and the author's laboratory.