05. X–1   COMPUTER SIMULATION OF PHASE TRANSI-
TIONS (CRYSTALLIZATION, SOLUTION ETC.). By
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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 ob-
tained 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. Be-
sides the field and the energy of the ensemble
other parameters such as the energy of the in-
dividual 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 provi-
ded either analytically or by providing discre-
te values. Presently only two dimensional pro-
cesses are considered, but the procedure does
not restrict to expansion to a third dimension.
"Crystals" up to 500 components have been pro-
cessed. By appropriate choice of input parame-
ters 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 distor-
tion 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 commen-
surate (or lock-in) phases, characterized by a polari-
zation wave of wave-vector $q_\delta = \delta b^*$. Neutron diffraction
experiments, at ambient 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 incom-
mensurate (0.115<δ<0.141) and ferroelectric (δ=0)
phases. Two other commensurate phases with δ=1/7 and
δ=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 δ=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 δ=1/8 commensurate lock-in
phase can be induced by an applied electric field.

05. X–3   TAILORING OF COMPOSITE SENSORS. By R. E.
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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 mate-
rial "figure of merit". Symmetry, connectivity, per-
colation, 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
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A twin is a regular oriented intergrowth of two
or more (congruent or enantiomorphic) individu-
als of the same crystal species. It is charac-
terized 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, ferromagne-
tic, and ferroelastic crystals (ferroic tran-
sitions). Mechanical twinning due to stress
includes ferroelasticity. Of particular inte-
rest 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 lat-
tices (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 'trans-
lation 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 micros-
copy, 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 boun-
daries will be given, with emphasis on minerals
and related compounds, both from the literature
and the author's laboratory.