As the potential functions prove to be adequate for these calculations the single vacancy parameters have been computed for adamantane with a <110> direction of jump. The calculated value of the formation energy E_f for a single vacancy is equal to 64.5 KJ mole^{-1}. It is close to the value of 70 ± 10 KJ mole^{-1} measured by positron annihilation for the vacancy formation energy in adamantane (D. Lightbody, J.N. Sherwood and M. Eldrup, Chem. Phys. Letters (1980) 70, 3, 487). The calculation of the migration energy E_m shows clearly that the relaxation around the migrating molecule exchanging with the vacancy is mainly due to molecular rotational movements. The value of E_m : 90 KJ.mole^{-1} yields an activation E_D of 154.5 KJ.mole^{-1} for self diffusion by a single vacancy mechanism. This value of E_D is in good agreement with the results obtained by N.M.R. and tracers experiments. So one may conclude that the self diffusion mechanism in adamantane is a single vacancy one, but it is necessary to have informations about other vacancy type defects and divacancy parameter calculations are in progress.

11.3-04   THE MECHANISM AND ENERGETICS OF DIFFUSION IN LANTHANUM TRIFLUORIDE. By J.R. Walker and C.R.A. Catlow, Department of Chemistry, University College London, 20 Gordon Street, London WC1H OAJ, U.K.

We present the results of a study into the formation and diffusion of defects in the tysonite-structured compound lanthanum trifluoride (Cheetham, A.K. et al., Acta Cryst. (1976) B32 94), which is shown by specific heat data to have an exceptionally high defect concentration at elevated temperatures. The method of study which we have adopted is a combination of theoretical techniques and single crystal neutron diffraction. In the course of our simulations we have modelled the LaF$_3$ crystal as an ensemble of ions interacting via long-range Coulombic forces and a short-range pair potential of Buckingham form. The formation and migration of defects in this ensemble of ions is then simulated by a combination of static (Norgett, M.J., AERE R7650, United Kingdom Atomic Energy Authority) and molecular dynamics techniques (Walker, J.R. in preparation). These simulations, together with the results of a single crystal neutron scattering experiment conducted at the Institut Laue-Langevin, Grenoble, France, have allowed us to identify unambiguously the sites responsible for, and the energetics of, anionic conduction in lanthanum trifluoride. The results provide a good illustration of the concerted use of theory and experiment in studying the high temperature disorder in inorganic solids.

11.3-05   THE FORCE LAW FOR DISLOCATION-POINT DEFECT INTERACTION AND DISLOCATION KINETICS STUDIES BY ACOUSTIC TECHNIQUES. By S.P. Nikanorov and B.K. Kardashev, A.F.Ioffe Physical-Technical Institute of the Academy of Sciences of the USSR, Leningrad, USSR.

Studies have been made of the amplitude dependent internal friction. A simultaneous study of the amplitude dependence of an alternating electric field arising in alkali halide crystals due to the oscillatory motion of charged dislocations was made as well.

Sets of dislocation internal friction amplitude dependences obtained at various temperatures make possible to present the effect of temperature on the stress required for unpinning dislocation segments of a certain length.

A correlation is found between the temperature dependence of an unpinning stress determined by internal friction technique and that of the yield stress values taken from the stress-strain curves. This correlation was established for LiF, NaF, NaCl nominally pure crystals; for LiF:Mg^{+2}, NaF:Ca^{+2} crystals and the layer "composites" prepared by a periodic intra-layer X-ray irradiation of LiF and NaF crystals, as well as for Al single crystals.

Th, results obtained enable us to build up a profile of the force law for the dislocation-point defect interaction determining both the amplitude dependent internal friction and the primary stages of plastic flow in crystals with a low Peierls barrier.

11.3-06   THE CHANGE OF REAL STRUCTURE DUE TO DISLOCATION STRESSES AND ITS EFFECT ON THE ELECTRICAL PROPERTIES OF SILICON SINGLE CRYSTALS. By V.I. Nikitenko, E.B. Yakimov and N.A. Yarykin, Institute of Solid State Physics, Academy of Sciences of the USSR, Chernogolovka, Moscow District, USSR.

The conditions of point defects practically always occur near immobile and moving dislocations alike, because this process leads to partial relaxation of dislocation elastic stresses, and consequently decreases the total crystal energy. If the concentration of these point defects is high enough, the complex centers can form effectively near dislocations even in the absence of these reactions away from the dislocations. If these complexes are electrically active, their influence on the electrical properties of crystals can exceed the direct dislocation effect due to the existence of unsaturated bonds in its core and of the specific field of dislocation elastic microstresses. The high temperature thermal treatment during plastic deformation or subsequent annealing leads to an increase in the rates of dislocation formation and the reactions of complexes. These result in a change of the spectrum of dislocation energy levels. In Czochralsky grown crystals with small dislocation density $(N_D \leqslant 10^7 cm^{-2})$, even a small change of temperature and duration of plastic deformation or subsequent thermal treatment can lead to a qualitative change of dislocation effect on the concentration of the charge carriers. The change in the spectrum of dislocation energy levels was studied by thermostimulated depolarization of both photo- and thermoelectric states in plastically deformed silicon and in dislocation p-n-junctions. The existence of the electric effect in dislocated silicon crystals is stipulated by increasing (by more than 14 orders of magnitude) the relaxation time of spatially inhomogeneous charge distribution produced by an electric field. Our inves-