As the potential functions prove to be adequate for these calculations the single vacancy parameters have been computed for adamantine with a <110> direction of jump. The calculated value of the formation energy \( E_f \) for a single vacancy is equal to 64.5 \( \text{kJ mole}^{-1} \). It is close to the value of 70 ± 10 \( \text{kJ mole}^{-1} \) 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 \( E_m \approx 90 \text{kJ mole}^{-1} \) yields an activation \( E_a \) of 154.5 \( \text{kJ mole}^{-1} \) for self diffusion by a single vacancy mechanism. This value of \( E_a \) is in good agreement with the results obtained by N.M.R. and tracer 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 divancy 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 of diffusion on 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 LaF₃ crystal as an ensemble of ions interacting via long-range Coulomb 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 FORGE LAW FOR DISLOCATION-POINT DEFECT INTERACTION AND DISLOCATION KINETICS STUDIES BY ACoustIC TECHNIQUES.** By O.P. Merkurov and B.K. Kardashev, A.P. 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 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 centres 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 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 Czochralski grown crystals with small dislocation density \( \left( N_d \approx 10^7 \text{cm}^{-2} \right) \), 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 changes in the spectrum of dislocation energy levels was studied by thermoelectromotive decomposition of both photo- and thermoelectric states in plastically deformed silicon and in silicon 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.