

As the potential functions prove to be adequate for these calculations the single vacancy parameters have been computed for adamantane with a $\langle 110 \rangle$ 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 $70 \pm 10 \text{ KJ mole}^{-1}$ 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 $E_m : 90 \text{ KJ.mole}^{-1}$ yields an activation E_D of $154.5 \text{ KJ.mole}^{-1}$ 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 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 0AJ, 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.

These 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 ($N_D \leq 10^7 \text{ cm}^{-2}$), 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-

tigations show that this method can provide information simultaneously about a number of deep dislocation energy levels in silicon single crystals. The results obtained by thermostimulated depolarization are compared with data obtained by traditional methods (Hall effect, spectral dependence of photoconductivity).

It is shown that a slip plane assumes the role of a new two-dimensional defect of the revealed structure. This two-dimensional defect is made up of an assembly of point-defect complexes which are formed in dislocation conditions and are left in the slip plane. This is caused by a smaller diffusion coefficient compared to that of the point defects. It is observed that part of point defects gathered by dislocation are transported by pipe diffusion to the crystal surface where they are fixed as microprecipitates. The dependence of the observed effects on temperature and duration of deformation, on thermal treatment conditions, and on impurity contents of the crystals has been investigated.

11.3-07 DISLOCATION MOBILITY IN SEMICONDUCTOR CRYSTALS IN CONNECTION WITH THEIR REAL STRUCTURE. By I. E. Bondarenko, V. I. Nikitenko, B. Ya. Farber, Institute of Solid State Physics Academy of Sciences of the USSR, Chernogolovka, Moscow distr., USSR.

The investigations of the dislocation mobility in covalent crystals have revealed essential contradictions between the experimental data and predictions of the theory of the dislocation mobility in a deep Peierls potential of the ideal lattice. To study the cause of the revealed discrepancies an investigation of dislocation mobility in Ge and Si has been made under conditions permitting one to select the contribution of the dislocation splitting and dislocation-point defects interaction to the movement of dislocations. The measurements of the dislocation velocity in Ge have been fulfilled within a high temperature range $T > 600^\circ\text{C}$, that have not been studied earlier. It has been found that at low stresses the activation energy for the dislocation motion decreases essentially as compared with the low temperature range. The analysis has shown that the behaviour of the temperature dependence of the velocity cannot be described in terms of the theoretical models based on the assumption of the influence of point defects on kink migration, even if the dislocation splitting and the reduction of point defects concentration with rising temperature are taken into account. It was, however, observed, that the results can qualitatively be described by these models at low temperature $T < 600^\circ\text{C}$. Investigating the dislocation mobility dependence in Si and Ge on the conditions

of bringing the dislocation to the starting position, it turned out possible to reveal a number of essential characteristics of dislocation-point defects interaction. It has been shown that the dislocation mobility is determined not only by the initial impurity contents of the crystals, but by point defects collected by the dislocation during its motion. The concentration and structural state of such defects depend on the dislocation velocity, pathway length and thermal treatment conditions upon bringing the dislocation to the starting position. It has been found that impurities collected by the dislocation as well as complexes, forming from gathered impurities in the field of dislocation microstresses, determine the kink mobility and give rise to a decrease of dislocation velocity and to the appearance of the starting stress. The high temperature data obtained for Ge can be explained under the assumption of the structural state changes of collected impurities occurring in some temperature range. It has been found that the dislocation velocity increases during the movement of the same dislocation as its motion direction is reversed. It is shown that this effect is not connected with the different resistance to the motion of partial dislocations, from which the perfect dislocation consists, but it is probably stipulated by the influence of the change in point defects state in the glide plane swept off by dislocation. The results obtained necessitate an account of the various manifestations of dislocation-point defects interaction in a real crystal leading to the essential change of the potential relief of the crystal lattice in the volume adjacent to the dislocation and in the region swept off by moving dislocation.

11.4-01 THE DETERMINATION OF DEBYE CHARACTERISTIC TEMPERATURES OF CRYSTALS FROM X-RAY POWDER DIFFRACTION INTENSITIES. By S. S. Lu and J. K. Liang, Institute of Physics, Academia Sinica, Beijing, China.

The methods of determining Debye characteristic temperatures from X-ray powder diffraction intensities have been fully discussed.

In the case of homogeneous and isotropic crystals, if the natural logarithms of the ratios of calculated intensities to observed intensities $\ln(I_{\text{calc.}}/I_{\text{obs.}})$ of all diffraction lines are plotted against $\sin^2\theta/\lambda^2$, the slope of the straight line obtained should give $2B$, where B is the Debye parameter.

For anisotropic crystals, if $\ln(I_{\text{calc.}}/I_{\text{obs.}})$ of $(hk0)$ and $(00l)$ reflexions are plotted against $\sin^2\theta/\lambda^2$ respectively, the two straight lines obtained should intercept at the same point on the ordinate axis. The slopes of the straight lines should give $2B_{\parallel}$ and $2B_{\perp}$, where B_{\parallel} and B_{\perp} represent the Debye parameters parallel and perpendicular to the principal axis respectively.

For inhomogeneous crystals, if there are two kinds of atoms (a) and (b) in the crystal, then the diffraction lines in the Debye-Scherrer photograph may be classified into two categories: the structure factors are either the sum F^S or the difference F^D of the structure factors of the respective atoms. Owing to the fact that both F^S and F^D are functions of $\sin\theta/\lambda$, so, if the observed values of $F^S_{\text{obs.}}$ and $F^D_{\text{obs.}}$ are plotted against $\sin\theta/\lambda$, two smooth curves should be obtained. From these two curves the corresponding values