11.3-01 DISLOCATIONS IN DEFORMED IRON WHISKERS. By
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Iron whiskers produced by hydrogen reduction of ferrous chloride were studied by X-ray transmission topography to obtain information on grown-in dislocations and dislocations in deformed iron whiskers. In as grown iron whiskers a regularity was observed in the distribution of dislocations. In whiskers with the same growth direction dislocation lines are parallel and have identical orientation in all specimens. The grown-in dislocations are of the screw type and lie in {110} or more rarely in {112} planes and their Burgers vectors are parallel to <111> directions. In order to observe in situ the evolution of the dislocation configuration in the whisker under the stress, the tensile machine was applied (Ch. G'sell and G. Champier, Phil. Mag. 41A (1980) 447). During tensile test examination of iron whisker grown-in dislocations do not change their positions but they act as sources for multiplication of dislocations. Propagation of the dislocations starts from the places of the highest density grown-in dislocations. Dislocations introduced during deformation have the same type as grown-in dislocations. After a certain stage of deformation a change of orientation of the crystal lattice of the whisker takes place.

11.3-02 DEFECT GENERATION IN LEC-GaP CRYSTALS. By
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During the last ten years the perfection of LEC-GaP has been extensively studied. Using preferential etching as the diagnostic tool, various etch pits have been observed. LEC-GaP has been analysed with TEM by Dupuy and Lafeuille (J.Crystal Growth (1975) 31, 244), de Kock et al. (J.Crystal Growth (1977) 41, 13), and Umeno et al. (Phil.Mag. (1979) A39, 183). The experimental results presented in these papers show that S-doped and undoped LEC-GaP investigated contains high concentrations (up to 10^{12} cm^{-3}) of generated defects which mainly appear in configurations such as faulted, perfect and polygonal loops and (semi) coherent precipitates. The loops are always associated with tetrahedron-formed precipitates. However, the nature of those precipitates could not be analytically identified, which fact led to controversial assumptions. In this paper, the results of TEM, EPMA and X-ray investigations of Te- and S-doped LEC-GaP are presented. Fig. 1. shows a schematic diagram of our growth model for the defects observed. Impurities may play a role in loop generation. In GaP (stacking-fault energy 45 mJ/m^2, Gai and Howie Phil.Mag. (1974) 30, 939) the prismatic Frank-type loops (a) on {111} planes with Burgers vector b = a/3 ⟨111⟩ are formed initialy. Some of these loops can be converted to perfect loops (a') by nucleation of Shockley partials (their conversion is stress-aided). The impurities begin to precipitate on the prismatic loop. The grown precipitate yields a stress field around it. To relieve the stress, the loop expands. Perfect loops on or near {111} plane (a') with b = a/2 ⟨110⟩ rotate during the expansion (b',b") onto {110} plane (c',c") so as to minimize the dislocation line energy. The precipitates nucleate on the dislocation line. Their growth (in {111} plane) occurs when they are pinned to the dislocation line only. However, as a large precipitate cannot move with the dislocation, it remains inside the loop when the latter subsequently expands and nucleation and growth of new precipitates on the dislocation line take place. The final stable defects (c, c', c") appear as faulted loops (c) on {111} plane (b= a/3 ⟨111⟩), and edge dislocation loops on or near {110}plane (b= a/2 ⟨110⟩). The latter are polygonal (c") or near-circular (c'). Precipitates associated with faulted loop are in the {111} loop plane, while those associated with perfect (c') or poligonal (c") loops are in or above the plane of the loop. The loops have interstitial-type character. The shape of etch precipitate is a tetrahedron formed by {111} GaP planes. The precipitates were identified as a compound consisting of Si, O and P (possibly also Ga, but the problem is not solved yet). The interplanar distances, obtained from the tetrahedron-formed precipitates, were: 4.14, 3.85, 3.74, 2.82, 2.56, 2.49, 1.92 Å. High concentrations of Si and O impurities seem to be introduced during the synthesis process (if quartz tubes and high temperatures were used). Depending on the concentration and distribution of these impurities, their interaction with dopant elements, and the quenching conditions in LEC growth process, different forms of defects appear.

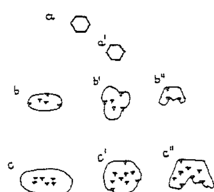

Fig. 1.

11.3-03 CALCULATION OF VACANCY TYPE DEFECT PARAMETERS FOR THE HIGH TEMPERATURE PHASE OF ADAMANTANE. by
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Point defect characterization is of importance to discuss several physical properties of crystalline solids. The calculation of the parameters for the various possible point defects is interesting in order to compare with the self diffusion measurements and to determine which kind of point defect is responsible of the diffusion process. Such a calculation is in progress for vacancy type defects in the high temperature phase of adamantane. In the particular case of O.D.I.C. crystals like adamantane, it is necessary to take into account not only the translational but also the rotational movements of the molecules to describe the relaxation around the point defects.
The calculation of the point defect formation and migration energies requires the computation of the lattice energy of the crystal with and without defect. The minimization of this lattice energy by rotating and translating the molecules neighbouring the defect yields the relaxation. The atom-atom potential method is used to calculate the lattice energies with (6-exp) potential functions and sets of parameters due to Williams (J. Chem. Phys.(1966) 45, 3770). The lattice sums and the minimization procedure are similar to those used in the PCK6 computer program (D.E. Williams, Acta Cryst.(1972) A28, 629).
The potential parameters have been checked for adamantane by computing the lattice energy E_C, the bulk modulus B and the barrier height for molecular rotation U_r, the agreement with experimental values is very good.

	E_C(KJ.mole^{-1})	B(Nm^{-2})	U_r(KJ.mole^{-1})
calculated	64.5	5.4 10^9	12.7
experimental	58-59.5-62.5-63.5	5.6 10^9	11.6-12.5

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