11.3-01 DISLOCATIONS IN DEFORMED IRON WHISKERS. By M. Surowiec*, Z. Bojarski* and G. Champier°, °Ecole des Mines, Nancy, France and *Silesian University, Katowice, Poland.

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 E.Mizera, K.Godwod and T.Warmiński, Institute of Physics, Polish Academy of Sciences, Warsaw, Poland.

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^{17} 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.

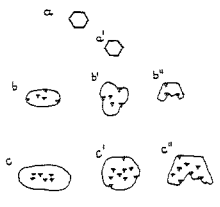

Fig. 1.

11.3-03 CALCULATION OF VACANCY TYPE DEFECT PARAMETERS FOR THE HIGH TEMPERATURE PHASE OF ADAMANTANE. by M. MEYER, L.P.M.-C.N.R.S. 1 Place A. Briand, 92190 Meudon Bellevue, France.

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