

**07.6-01** THE ABSORPTION AND DESORPTION OF HYDROGEN AND DEUTERIUM IN  $Mg_2Ni$ . By A.F. Andresen, E. Andersen and K. Pettersen, Institute for Energy Technology, Kjeller, Norway.

Neutron diffraction offers a unique possibility of studying structural changes during the absorption of gases under high pressure and temperature. This we have utilized to study the structural transformations and the kinetics in the absorption and desorption of hydrogen and deuterium in  $Mg_2Ni$ . The processes limiting the rate of absorption at the different compositions have been identified and characteristic differences between the absorption of hydrogen and deuterium have been found.

The hydride  $Mg_2NiH_4$  shows an allotropic transformation between a high temperature cubic structure and a low temperature monoclinic structure. The transition is connected with a hysteresis and shows a marked isotope effect. For  $Mg_2NiH_4$  we find the transition at  $237^\circ - 246^\circ C$  and for  $Mg_2NiD_4$  at  $229^\circ - 238^\circ C$ .

be monodispersed into rectangular groups of 25 overlapped primary  $C_6$  rings and by intramolecular interaction become 5 times superposed in thickness making up  $20.5 \text{ \AA}$ ; this results as equidimensional parallelepipedon of crystallizing unit consisted of 1500 C atoms and bounded by (111), (110) and composite (100) planes exposing to-and-fro shifted elements. The X-ray photoelectron spectrogram of the M-C film containing about 32 wt.% Ni within  $200 \text{ \AA}$  from the interface with diamond is not of zero-valent Ni but in a valence state of  $Ni(II)d^8$ .

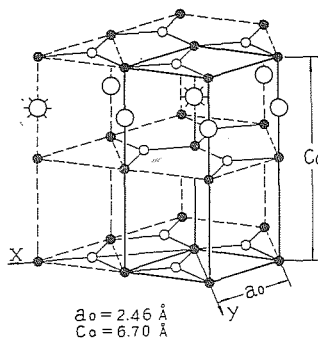


Fig. 1. The structure of hexagonal graphite intercalated with Ni or M atoms in CCMCCM sandwich (without showing the puckering and shifting of C lattice).

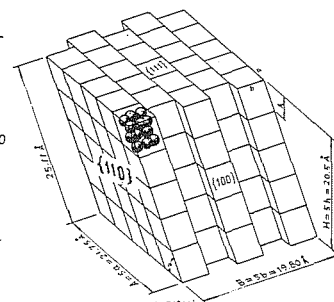


Fig. 2. The growth unit of synthetic diamond.

**07.7-01** THE ROLE OF SOLVENT-CATALYST ON PROMOTION OF GRAPHITE TO DIAMOND TRANSITION. By Zhang Yuan-long (Chang Yuan-lung) and Li Da-ming, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, CHINA.

The rules of deformation of graphite lattice in metal-carbon solvent film and the variation of metallic valence promoting the graphite to diamond transition have been investigated. Carbon atoms in graphite may be either repeated themselves in successive layers, indicated as C' (●) in Fig. 1, or superposed in every other layer (and every third layer for the rhombic structure) as C'' (○). Under high temperature and ultra-high-pressure, the invasion of melted metals of group VIII (M) into the interlayer spacings of graphite (C) should be sequenced as CCMCCM. The carbon atoms, C'' occupy octahedral holes in the close-packed metal lattice, while the C' lie between another C' and M atoms (○), therefore, the carbon layers are puckered. As zero-valent metals do not form M-C bond, only geometrical alignment along C'-C''-M-C'-C''-M are preserved. When Ni atoms (○) making up as much as 1/3 of M are promoted to the valence state  $Ni(II)d^8$  (○), then  $sp^3$  hybridized, however octahedral coordinated, delocalized, covalent complexes are formed in layers. The central metal d electrons are oscillatory delocalized onto the ligand atoms C'', while the carbon layers are even over-puckered by  $10^{25}$  compared with the bond angle  $109^\circ 28'$  of diamond. Dimers of diamond are formed and dissociated during mutual-approach of the double C layers. Fig. 2, shows the crystallizing unit of synthetic diamond composed of rectangular dimers superposed into parallelepipedon, for the minimization of surface free energy, the height, H, and the sides of the base, A and B, should be  $nh$ ,  $na$  and  $nb$ , while  $h=4.10 \text{ \AA}$ ,  $a=4.35 \text{ \AA}$  and  $b=3.96 \text{ \AA}$  are the dimensions of a primary parallelepipedon inscribing a pair of overlapped  $C_6$  rings. The postulation of  $n=5$  is made in accordance with the fact that the step height of the growth spiral originating from a dislocation on (111) plane has been determined to be  $20 \text{ \AA}$  (communicated by Liu Guang-zhao). Therefore, within certain P-T region the dimers may

**07.8-01** STRUCTURE OF A MIXED CHALCOGENIDE OF INDIUM WITH APPROXIMATE COMPOSITION  $In_{2.03}X_3$  (X = S, Se AND Te). By C. Svensson and J. Albertsson. *Inorganic Chemistry, Chemical Center, University of Lund, P.O.B. 740, S-220 07 Lund, Sweden.*

The black title compound was synthesized from the pure elements and an analysis indicated the composition S:Se:Te  $\approx 1:2:3$  (Titze (1981) to be published). A number of semiconducting indium chalcogenides have been described but this seems to be the first one containing all three of S, Se and Te. It is rhombohedral with space group  $R\bar{3}$  and lattice constants  $a = 14.0028(10)$  and  $c = 35.228(5) \text{ \AA}$  (hexagonal axes). The structure was solved and refined using 4535 observed X-ray diffraction data.

A feature of several indium chalcogenides which has not been appreciated until now is the appearance of a small amount of univalent indium with positional disorder. The present compound should be formulated  $In_{1-x}^{I}In_{25+x}^{III}X_{38+x}$  with  $x \approx 0.3$ . The In(I) atom is located just off a point with  $\bar{3}$  symmetry in an enlarged octahedral interstice and coordinated from one side by three Te. One of the 25 In(III) has octahedral coordination (by six Te atoms) and the others are tetrahedrally coordinated. The structure, which is a three-dimensional network, is pseudo-symmetric such that the c-axis is doubled. The In(I) atoms correspond to the octahedral In(III). The cell with half the c-axis is a pseudocube with  $a = 10.0 \text{ \AA}$  and  $\alpha = 89.0^\circ$  (rhombohedral axes) but the structure is not of the spinel type. The tetrahedral In(III)-X bonds range from  $2.557(3)$  to  $2.825(2) \text{ \AA}$ ; the octahedral In(III)-Te is  $2.975(2) \text{ \AA}$  and In(I)-Te is  $3.250(5) \text{ \AA}$ .