07.6-01 THE ABSORPTION AND DESORPTION OF HYDROGEN AND DEUTERIUM IN Mg,Ni. By A.P. Andersen, 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 has enabled us to study the structural transformations and the kinetics in the absorption and desorption of hydrogen and deuterium in Mg,Ni. The process 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,NiH 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,NiH we find the transition at 237 °C to 246°C and for Mg,NiD₄ at 229°-230°C.

07.7-01 THE ROLE OF SOLVENT-CATALYST ON PROMOTION OF GRAPHITE TO DIAMOND TRANSITION. By Zhang Yuan-long (Chang Yuan-lung) and Li Xian-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' (S) in Fig. 1, or superposed in every other layer (and every third layer for the rhombohedral structure) as C" (O). Under high temperature and ultra-high-pressure, the invasion of related metals of group VIII [M] into the interlayer spacings of graphite (S) could be sequenced as CaCO₂. The carbon atoms C" occupy octahedral holes in the close-packed metal lattice, while the C' lie between another C" and H atoms (O), therefore, the carbon layers are puckered. As zero-valent metals do not form h-c bond, only geometrical alignment among C'(~)-H:-C"-H:-C"-H:-C' is preserved. When H₂ atoms (O) making up as much as 1/3 of H are promoted to the valence state Ni(II)H₄ (O), then sp³ hybridized, however octahedral coordinated, delocalized, covalent complexes are formed in layers. The central metal d electrons are oscillatory localized onto the ligand atoms C" while the carbon layers are even over-puckered by 1°-2° compared with the bond angle 109°-28° of diamond. Planes 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 minimisation of surface free energy, the height, H, and the sides of the base, A and B, should be nh, na and n b, while nh=10.1 Å, na=3.55 Å and n b=3.96 Å are the dimensions of a primary parallelepipedon inscribing a pair of overlapped H₂ rings. The postulate of n=3 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 Å (communicated by Liu Guan-shao). Therefore, within certain P-T region the dimers may be monodispersed into rectangular groups of 25 overlapped primary H₂ rings and by intramolecular interaction become 5 times superposed in thickness making up 20.5 Å; this results as edgewise-plane 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 spectrograms of the H₂ film containing about 32 wt.% Ni within 200 Å from the interface with diamond is not of zero-valent Ni but in a valence state of Ni(II)H₄.


The black cubic compound was synthesized from the pure elements and an analysis indicated the composition S:Se:Te = 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 R3 and lattice constants a = 14.0028(10) and c = 35.238(5) Å (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 Inₓ₂Sₓ₂Teₓ₁₋ₓ (1-x) with x = 0.3. The In(I) atom is located just off a point with 3 symmetry in an enlarged octahedral interface and coordinated from one side by three Te. One of the 25 In(I) is octahedral coordinated (by six Te atoms) and the others are tetrahedrally coordinated. The structure, which is a three-dimensional network, has pseudo-symmetric such that the a-axis is doubled. The In(I) atoms correspond to the octahedral In(III). The cell with half the a-axis is a pseudocube with a = 10.0 Å and a = 89.0° (rhombohedral axes) but this structure is not of the spinal type. The tetrahedral In(III)-X bonds range from 2.557(3) to 2.825(2) Å; the octahedral In(III)-Te is 2.975(2) Å and In(I)-Te is 3.250(5) Å.