

sistent with the postulated strong metal - non metal interactions in this compound.

In contrast, no significant distortions from spherical symmetry are observed around the C atom sites.

A AgK_{α} data set is currently being measured to confirm these features.

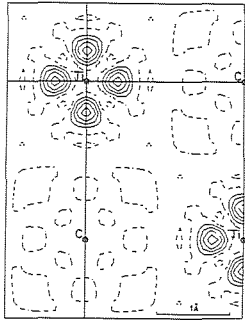


Fig. 1 : Deformation density of TiC in the (100) plane. Ti and C atoms sites, symmetry is $m\bar{3}m$. Contour intervals at $0.1 e/\text{\AA}^3$. Zero and negative contours broken.

* The crystal was kindly provided by Dr. Politis, at the Kernforschungszentrum Karlsruhe.

06.2-16 EXPERIMENTAL STRUCTURE FACTORS OF ZnSe. By R. Uno, Y. Ohgiri, M. Nakajima and J. Ishigaki, College of Humanities and Sciences, Nihon University, Sakurajosui, Setagaya-ku, Tokyo 156, Japan.

The experimental structure factors of ZnSe were obtained from an X-ray measurement performed by P.M. Raccan et al (Phys. Rev. 148(1966) 904). Among the factors, those of the difference lines, where $h+k+l=4n+2$, are appreciably larger than those theoretically calculated by using self-consistent OPW model (Phys. Rev. B1(1970) 756).

Since the difference lines overlap with the tail of stronger lines, separation of the difference lines from the adjacent stronger lines was made, in the present work, according to the profile-fitting method, by the use of parameters determined from well-separated lines. Preliminary results shows that the structure factors of the difference lines at low Bragg angles, such as F(200) and F(222), are not larger than the theoretical values. This will give considerable influence to the solid state effect on the electron distribution of atoms in ZnSe.

06.2-17 THE X-RAY STUDY OF ELECTRON DENSITY DISTRIBUTION IN REAL SPACE IN IONIC-COVALENT STRUCTURES $A''B''$ AND ITS INFLUENCE ON SPECTRUM CHARACTERISTICS. By J. Jakimavichus, R. Purlys and A. Shirvaitis, Faculty of Physics, Vilnius University, Vilnius, Lithuania USSR.

Electron density distribution of valence electrons in real space and its influence on effective ion charges, lattice potential and energy level components of zone structure electron spectra have been investigated in cubic (ZnS, ZnSe, CdTe) and hexagonal (CdS, CdSe, ZnO) structures. Lattice electron density and ion distributions have been obtained by Fourier transform of structure amplitudes and form factors, measured by X-ray from CuK_{α} . For the construction of potential components and calculation of energy levels the technique of (J. Jakimavichus, J. Batarūnas, Phys. Molecules, (1976) Nr. 2, 61) has been used. Valence electron density increase in the regions of principal maximums of valence electrons wave function have been shown in crystals. The electron density change in crystals was found to be bigger compared with its theoretical investigation taking into account atom ionization and excitation to valence state. This change causes the increase of effective ion charges and the decrease of structure amplitudes and potential components (200) and (011) in cubic and hexagonal structures respectively. This, in its turn, conditions the decrease of conductivity zone lower levels and diminution of the forbidden zone width. The reduction of conductivity zone levels has been shown to become smaller with the increase of bond ionicity of the investigated compounds $A''B''$.

06.2-18 NEUTRON AND X-RAY DIFFRACTION STUDY OF THE CRYSTAL STRUCTURE OF SiP_2 . By T. Chattopadhyay, and H.G.v.Schnering, Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 7000 Stuttgart 80, Federal Republic of Germany

Neutron diffraction data have been collected from SiP_2 single crystal with pyrite structure at 60, 120 and 293 K. The positional and thermal parameters have been obtained at these temperatures by refining them with these intensity data. The conventional agreement factors for these refinements are $R=0.044$, 0.060 and 0.076 at 60, 120 and 293 K respectively. The variation of the structural parameters with temperature have been studied and discussed. Accurate X-ray diffraction data have been collected from a spherical SiP_2 single crystal at 293 K up to $\sin\theta/\lambda=1.2 \text{\AA}^{-1}$. Calculations of valence and deformation densities } X-N are in progress and will be presented at the meeting. The isotropic temperature parameters of Si and P atoms obtained from neutron diffraction studies vary linearly with temperature. The mean square vibrational amplitudes of Si and P atoms are practically the same at low temperature, but at the room temperature the mean square amplitude of Si atom is found to be larger than that of P atom.