06.2-2   ELECTRON   DEFORMATION   DENSITY   IN ALPHA - BORON. By G. Will, B. Kiefer, Mineralogical Institute, University Bonn, West Germany; B. Morosin, Sandia National Lab., Albuquerque, NM USA; and   G. Slack, General Electric Res. and Dev., Schenectady, NY USA.

The bonding features of alpha-boron were studied using electron density analysis procedures, including valence and deformation density maps and multipole refinement on MoKalpha data.

Refinement with 349 data and spherical atomic scattering factors resulted in R = 6.2%, while using only the high order data gave R = 2.2%. Therefore substantial electron density due to bonding remains. Deformation and valence density maps were calculated and the final structure was analyzed by so-called multipole refinements, yielding R = 1.19%.

The density distribution shows a small, rather uniform charge accumulation in the B-B bonds in the icosahedra and similar small charge between the icosahedra along the three center or "delta" bonds. A comparative large charge accumulation is found on the B-B bonds connecting the icosahedra along the c-axis.

06.2-3   ELECTRON DENSITY DISTRIBUTIONS IN GAP,GAAS AND GASB.   By R.Uno, K.Yukino, J. Ishigaki and H.Ozawa,   College of Humanities and Sciences, Nihon University, 3-25-40, Sakurajosui, Setagaya-ku, Tokyo 156, Japan.

Crystal structure factors were obtained from fine powder samples on GaP (J. Appl. Cryst., 1975,8, 578), GaAs (J. Phys. Soc. Jpn.,1970, 28, 437) and GaSb (Acta Cryst., 1984, 40, C-164).   Electron density distribution was investigated again by the difference Fourier synthesis with an assumption of unharmonic thermal vibration.
The atomic potential is assumed to be
$$V(u)=V_0+(1/2)\alpha u^2+\beta u_1 u_2 u_3,$$
where $\bar{u}(u_1,u_2,u_3)$ is the displacement of an atom,since these crystals have the zincblende structure.   Parameters α and β were estimated in 5 digits along with the scale factor, on condition that an average value of $\Delta\varrho(r)$ should be minimum. The number of electrons in a sphere at the center of chemical bond in the map of $\Delta\varrho(\bar{r})$, was calculated against the sphere radius.   The maximum values of electron number were obtained as 0.055 for GaP, 0.18 for GaAs and 0.47 for GaSb.   Several linear relations were obtained between these numbers and effective charge from infrared reflection, static dielectric constant and effective atomic charge estimated by W.A. Harrison ("Electronic Structure and the Properties of Solids", W.H.Freeman and Co.,1980, p. 124).   These linear relations show that the electron number in the $\Delta\varrho(r)$ sphere can be a measure of the covalency of the chemical bond in the three crystals.

06.2-4   THE ELECTRON DENSITY DISTRIBUTION IN CALCIUM-METABORATE, Ca(BO$_2$)$_2$. By A. Kirfel Universität des Saarlandes, FR Kristallographie D-6600 Saarbrücken, Federal Republic of Germany

The room temperature electron density distribution in Ca(BO$_2$)$_2$ has been studied by X-ray diffraction experiments on two crystals, I and II, up to $\sin\theta/\lambda = 0.80$ Å^{-1} and 1.16 Å^{-1} respectively. Conventional structure refinements yielded weighted R-values of 0.025/ 0.021 for 603/ 1577 observed reflections. Data set II was used for high-order refinements in order to assess positional and thermal parameters least biased by bonding effects and to estimate a best scale factor. Rigid pseudoatom multipole expansions up to hexadecapoles resulted in final agreement factors $R_w = 0.0064/ 0.0088$ which represent highly significant improvements of the fit with observations. Parameters derived from the multipole refinements of both data sets were used to calculate dynamic and static deformation density distributions as well as deformation potential distributions in interesting sections of the structure. The choice of the resolution of the Fourier synthesis is shown to affect $\Delta\varrho(r)$, especially around the nuclear positions. The observed charge distributions are discussed in terms of chemical bonding in calcium-metaborate and in comparison with an earlier study on LiBO$_2$ (Kirfel, A., Will, G., Stewart, R.F., Acta Cryst., 1983, B39, 175-185). In addition,spherical charge integrations around Ca and B served to establish formal ionic radii and charges of the cations. All relevant results indicate predominantly ionic interaction between Ca(2+) and the (BO$_2$)$^-$ anions (of metaboric acid) which polymerize to endless chains of BO$_3$-triangles.

Crystal data: M = 125.70, a = 6.2046(3), b = 11.5865(7), c = 4.2747 Å, V = 307.31(6) Å^3, space group Pnca, Z = 4.
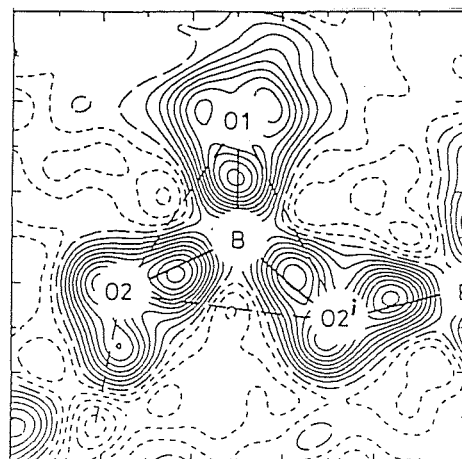
Dynamic deformation density in the BO$_3$ plane, s(max) = 0.80 Å^{-1}, contours at 0.05 eÅ^{-3}, zero contour broken, negative contours dashed.