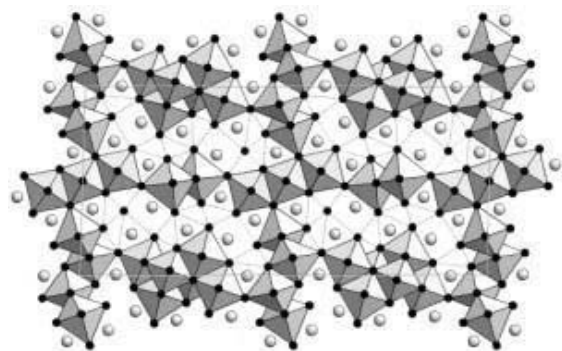


s5.m1.p3 **Crystal structure of $Ti_{45}Se_{16}$ Redetermined from Electron Diffraction Data.** T.E. Weirich, *Darmstadt University of Technology, Materials Science, Petersenstr  e 23, 64287 Darmstadt, (Germany).*
 Keywords: electron crystallography, mineralogy.

The metal-rich compound $Ti_{45}Se_{16}$ is one component in a polyphasic sample obtained from high-temperature synthesis. Due to the lack of large single crystals the structure was originally solved by crystallographic image processing from high resolution electron microscopy images [1]. The sample was recently reexamined by selected area electron diffraction in a 300 kV Jeol 3010UHR transmission electron microscope. A data set of 1047 crystallographically non-equivalent $h0l$ reflections (crystallographic resolution about 0.6  ) was obtained by quantifying diffraction patterns recorded on EM film. The structure of $Ti_{45}Se_{16}$ was solved by direct methods from the electron data using the program SIR97 [2]. Improved atomic co-ordinates were obtained by subsequent least squares refinement on the basis of the kinematical diffraction approximation using the program SHELXL97 [3].

The compound crystallizes in the monoclinic space group $C2/m$ (12) with lattice parameters $a = 36.534$, $b = 3.453$, $c = 16.984$  , $\beta = 91.73^\circ$. The structure of $Ti_{45}Se_{16}$ contains 23 titanium and 8 selenium atoms per asymmetric part of the unit cell ($Z = 2$). The refined atomic co-ordinates agree on average within 0.18   with the previous determined structure from high resolution electron microscopy images.

The structure of $Ti_{45}Se_{16}$ is at present the number eight in a line of metal-rich structures that was solved by quasi-automatic direct methods from two-dimensional selected area electron diffraction data [4, 5]. The result of this study shows again that complex heavy atom structures can be determined with high precision from electron diffraction even when only the simple quasi-kinematical approach is applied.



Structure model of $Ti_{45}Se_{16}$ (projection along the b axis) after LS refinement with electron data ($Ti = \bullet$, $Se = \circ$).

s5.m1.p4 **Electronic Structure CBN / C, Al, Mg, Si - Systems.** V.V. Ilyasov, *Don Technical University, Gagarin Sq.1, 344010 Rostov-on-Don, Russia.*
 Keywords: solid solutions, cubic boron nitride, electron structure.

With the coherent potential method of the multiple scattering theory [1] the electron structure the diamond-like system BN - (C, Al, Mg, Si) is calculated. Calculation partial local charges in the top part of valence band has shown, that the existing carry change from boron to nitrogen, observable in binary BN, changes a mark in BN-(C, Al, Mg, Si). In the last system nitrogen "transfers" boron, and the carbon acts in a role of the donor of electronic configurations boron and nitrogen. At doped the matrix c-BN the carbon or Al (Mg, Si) observes change of the form and energy situation of top of the valence band. It can be connected to downturn of symmetry in sublattice of nitrogen. The observable delocalization of partial local DOS of nitrogen, occurs without broadening N_s , p-band. Probably, it is caused by interaction the electrons s, p-impurity with basic s p³ - configuration BN, in result of which increase the desordered DOS in the valence band of the systems BN-C, Al, Mg, Si is observed.

Character of curve complete density of condition valence electrons of top of the valence band of a strip in considered systems speaks about presence of influence s, p-impurity on width of the band gap.

The area forbidden energy narrower than in c-BN and growth of DOS at a level Fermi conducts to essential change of major physical properties, that confirm accounts of conductivity from the first principles. These calculations are in a good correspondence with the experimental data.

- [1] Weirich, T. E. (1996). PhD Thesis, Universit  t Osnabr  ck, Germany.
- [2] Altomare, A., et al. (1999) *J. Appl. Cryst.* **32**, 115-118.
- [3] Sheldrick, G. M. (1998). SHELXL-97-2. Program for Crystal Structure Refinement. University of G  ttingen, Germany.
- [4] Weirich, T. E., Hovm  ller, S., Kalpen, H., Ramlau, R. Simon, A. (1998) *Crystallogr. Rep.* **43**, 956-967.
- [5] Weirich, T. E., Zou, X. D., Ramlau, R., Simon, A., Cascarano, G. L., Giacobozzo, C., Hovm  ller, S. *Acta Cryst.* (2000) **A56**, 29-35.

- [1] Ilyasov V.V., Nikiforov I.Ya., Ilyasov Yu.V / *J. Phys. IV France.-1997.-V.7.-P.C2-281.*