

s6.m1.p1 **The Pressure Effect of the Bulk Modulus Seen by the Charge Density in InX Compounds.** Y. AL-Douri and H. Aourag. *Physics Department, University of Sidi-Bel-Abbes, 22000 – Algeria. Fax : +(2137) 56 16 42. Email: yaldouri@hotmail.com*
 Keywords: semiconductors, bulk moduli, phase transitions.

The cationic part of the electronic charge densities of InX (X = Sb, As, P) compounds are calculated using the Empirical Pseudopotential Method (EPM) in order to obtain their bulk moduli. This factor has been calculated by means of our recent model¹. The pseudopotential form factors are adjusted by a nonlinear least-square method^{2,4}, in which all the parameters are simultaneously optimized under a definite criterion of minimizing the root-mean square deviation and for determining suitable charge densities. We show that the bulk modulus which reflects the hardness of the material can be seen and changed from the behavior of the bonding character under the pressure effect. The results are compared with experimental data with reasonable agreement.

s6.m1.p2 **Modern High-Pressure Measurements with a CCD Detector System.** L. Häming, M. Ruf, E. Hovestreydt *Bruker AXS GmbH, Product Support, Postfach, Karlsruhe.*
 Keywords: extreme conditions.

Area detectors and in particular CCD-based detectors have been around for quite while, but their advantage in the field of high-pressure single-crystal structure determination has been recognized only recently. In particular the fact that on a 3-axis goniometer virtually the same amount of data can be accessed, is now an accepted fact:

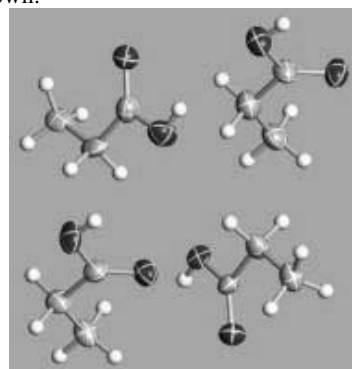
The area of reciprocal space accessible for X-ray examination is determined by the opening angles 2Ψ of the DAC and the opening angle Δ of the detector at a given distance.

For one orientation of the DAC, the accessible region is $\Sigma = 2\Psi - \Delta$ before the steel supports of the DAC start to obscure the detector. By a combination of Ω -scans using different orientations of the DAC in Φ , about one third of all reflections can be collected. A combination of just 8 runs with different detector settings and starting values for ω and ϕ covers 29% of estimated unique data for point group 1 with a mean redundancy of even 2. This coverage is just 2% less than what typically used to be accessible on conventional 4-circle geometry.



Sample (wh) and Diamond (gr) reflections Sample reflections

A huge advantage of now-a-days powerful twinning software is the fact that not only the sample under investigation, but also the 2 diamond anvils can be indexed and their orientation matrix obtained. This will allow the data processing software to obtain sample intensities which are corrected for possible overlap with diamond reflections. An example on how this affects data quality will be shown.



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