[2] I. Goncharenko, P. Cadavez-Peres, O. Makarova, T. Le Bihan, M. Mezouar, *Phys. Rev. B*, 2003, 68, 214418.
[3] N. Ashcroft, *Phys. Rev. Lett.*, 200492, 187002.
[4] I. Goncharenko, *High Press. Res.,* 2007, 27 183

MS22 O4

Single crystal studies of pure elements at high pressure

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Although the technique of high-pressure single-crystal diffraction has been used to study pure elements for many years [1], recent developments, such as improved diamond anvil cell design combined with CCD-equipped diffractometers and synchrotron sources, have allowed the structure solution of a number of complex new phases [2,3].
In this talk we will describe the technique of high-pressure single-crystal diffraction, and discuss its advantages and limitations. To Illustrate the power of the technique, we will present recent results on the full modulated structure of the incommensurate composite structure of Rb-IV, the structure of Ba-IVb and the structure of epsilon-oxygen [4].
Finally, we will describe our on-going development of techniques that will enable us to do combined high-pressure high-temperature single-crystal diffraction, and single-crystal diffraction at pressures of 50GPa and above.

[1] D. Schiferl, D. T. Cromer & R. L. Mills, Acta Cryst. (1981), B37, 1329-1332.
[2] M. I. McMahon, R. J. Nelmes & S. Rekhi, Phys. Rev. Lett. (2001), 87, 255502.
[3] R. J. Nelmes, M. I. McMahon, J. S. Loveday & S. Rekhi, Phys. Rev. Lett. (2002), 88, 155503.
[4] L. F. Lundegaard, G. Weck, M. I. McMahon, S. Desgreniers & P. Loubeyre, Nature (2006), 443, 201-204.

MS22 O5

Electric field induced lattice displacements in BiB_3O_6 crystals,

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Monoclinic BiB_3O_6 is a piezoelectric material with exceptional large piezoelectric coefficients [1]. At this material X-ray charge density analysis is highly affected by the huge difference in electronic numbers of constituting elements and by secondary extinction. However, measurements of intensity variation of selected Bragg reflection caused by an external high electric field provide information about the reorganization of atomic positions within the unit cell and subsequently about a change of chemical bonds [2]. For BiB_3O_6 we have measured several Bragg reflections under influence of an external electric field up to 20 kV/cm using synchrotron radiation. The measured change in angular positions of Bragg reflections is caused by the external piezoelectric effect. Measuring the respective peak shifts at three differently oriented crystal plates we have deduced all eight independent coefficients of the piezoelectric tensor of the material [3]. In addition, the intensity is changed due to the internal piezoelectric effect, i.e. the reorganization of atomic arrangement within the unit cell. Preliminary modelling suggested an effect less then 1%. However, tuning the probing wave length close to the absorption edge of Bi atoms we could measure the linear dependence of intensity variation as a function of the applied field at a [100] oriented crystal plate. Due to the small number of measured reflections we used a rough model for data interpretation, a displacement of rigid lattice of BO_3 units against the fixed Bi atoms. Normalized to E=1kV/mm we deduced a displacement vector $\Delta r = -(14,2\ a_1 + 47,5\ a_3)10^{-5}$, given in relative coordinates of the monoclinic system with $a_{1,2,3}$ as unit vectors. Since the external field was applied in direction $E = 0,146\ a_1 + 0,043\ a_3$ the displacement of the negatively charged BO_3 units are directed by an angle of about 75 degree with respect to the plane of positively charged Bi atoms.

[1] Haussühl, S.; Bohaty, L. ; Becker, P.: Piezoelectric and elastic properties of the nonlinear optical material bismuth triborate, BiB3O6. In: Appl. Phys. A 82 (2006),S. 495–502
[2] Gorfman, S. V.; Tsirelson, V. G.; Pucher, A.; Morgenroth, W.; Pietsch, U.: X-ray diffraction by a crystal in a permanent external electric field: electric-field-induced structural response in α-$GaPO_4$. Acta Cryst. A62 (2006) 1-10.
[3] S. Gorfman, O. Schmidt, U. Pietsch, P. Becker, L. Bohaty. X-Ray Diffraction Study of the Piezoelectric Properties of BiB_3O_6 Single Crystals (2007) Z. f. Krist, accepted