resulting large structural models (sets of thousands of atomic coordinates) were subjects of geometrical analyses: distributions of the number of first neighbours, as well as local angular correlations have been calculated. In the cases of molecular liquids investigated (like the case of liquid O_2), correlations between orientations of neighbouring molecules have been characterized.

[1] McGreevy R.L., Pusztai L., *Mol. Simul*.,1988, **1**, 359.

Keywords: high-pressure X-ray diffraction, diamond anvil cells, computer modelling liquids

MS68.28.4

Acta Cryst. (2005). A**61**, C88

X-ray Diffraction Study in Liquid Cs up to 9.8 GPa

Sara Falconi[a], Lars Fahl Lundegaard[a], Clivia Hejny[a], Malcolm McMahon[a] , [a]*School of Physics and Centre for Science at Extreme Conditions,The University of Edinburgh, Mayfield Road, Edinburgh, EH9 3JZ, United Kingdom.* E-mail: sfalconi@ph.ed.ac.uk

An x-ray diffraction study of liquid Cs at high pressure and temperature has been conducted in order to characterize the structural changes associated with the complex melting curve and phase transitions observed in the solid phases [1, 2, 3, 4]. At 3.9 GPa a discontinuity in the density of the liquid accompanied by a decrease in the coordination number from about 12 to 8 marks a change between simple and non-simple liquid regime [5].

The specific volume of liquid Cs, combined with structural analysis of the diffraction data, strongly suggest the existence of an electronic hybridization above 3.9 GPa similar to that reported on compression in the crystalline phase.

Further, *ab-initio* calculations with cluster of 264 atoms confirm the structural results obtained experimentally and reinforce the hypothesis of the electronic hybridization driven by compression of the solid and of the liquid.

[1] Kennedy G.C., Jayaraman A., Newton R. C., *Phys. Rev.*, 1962, **126**, 1363. [2] Jayaraman A., Newton R. C., McDonough J.M., *Phys. Rev.*, 1967, **159**, 527. [3] McMahan A.K., *Phys. Rev. B* , 1984, **29**, R5982. [4] Tsuji K. et al., *J. Non-Cryst. Sol.*, 1990, **117/118**, 72. [5] Falconi S. et al., *Physical Review Letters*, 2005, *in press*.

Keywords: caesium, high pressure, liquids

MS68.28.5

Acta Cryst. (2005). A**61**, C88

CdSb under Pressure: Compound Decomposition, New Phase Formation and Amorphization

Valentina F. Degtyareva[a], Olga Degtyareva[b], Russell J. Hemley[b], [a]*Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia.* [b]*Geophysical Laboratory, Carnegie Institution of Washington, USA.* E-mail: degtyar@issp.ac.ru

Application of high pressure offers wide possibilities to produce new materials in crystalline and amorphous states. The Cd-Sb alloy system has at ambient pressure one intermediate compound of equiatomic composition, CdSb, orthorhombic, space group *Pbca*, with 16 atoms in the unit cell. On pressure increase to 7.3 GPa, we observed a transition from CdSb-*oP*16 phase to a new state that is interpreted as a two-phase mixture of a simple hexagonal Sb-rich phase and a hexagonal close packed phase of (almost pure) Cd. At 8.4 GPa, lattice parameters are for the *sh* phase (space group *P*6/*mmm*) a = 3.066(1) Å and c = 2.860(1) Å, and for Cd-*hcp* phase (space group $P6_3/mmc$) a = 2.93(1) Å and c = 5.165(1) Å, close to those reported for pure Cd at this pressure. On pressure decrease, the two phase mixture state is observed down to 1 GPa and below 1 GPa, an amorphous phase is observed. The halos of the amorphous phase of CdSb sample correspond to Q_1=2.004 Å^{-1} and Q_2=2.953 Å^{-1}. The full width at half maximum of the halos corresponds to the correlation length 12-15 Å. The amorphous phases formed in binary alloys Zn-Sb, Cd-Sb and Al-Ge after pressure action are close to tetrahedral nets and correspond to nearly 4 el./atom composition [1,2].

Partial support from RFBR under grant 04-02-17343 is acknowledged.

[1] Belash I.T., Degtyareva V.F., Ponyatovskii E.G., Rashchupkin V.I. *Sov. Phys. Solid State*, 1987, **29**, 1028. [2] Degtyareva V.F., Belash I.T., Ponyatovskii E.G. *Phys. Stat. Solidi (a)*, 1991, **124**, 465.

Keywords: high-pressure phases, decomposition, amorphization

MS69 ELECTRON CRYSTALLOGRAPHY ON ORGANIC CRYSTALS AND BIOMOLECULES

Chairpersons: Hans Hebert, Ute Kolb

MS69.28.1

Acta Cryst. (2005). A**61**, C88

Electron Diffraction from a Beam of Laser-aligned Proteins: Progress Report

Uwe Weierstall, Dmitri Starodub, John C.H. Spence, Bruce Doak, *Department of Physics and Astronomy, Arizona State University, Tempe AZ 85287-1504, USA.* E-mail: weier@asu.edu

The use of diffraction patterns from aligned molecular beams has been proposed as an approach to the structure determination of proteins that are difficult to crystallize [1]. Polarized laser light is used to align the molecules in the beam. By cooling a beam of hydrated proteins to low temperature, sufficient alignment for diffraction purposes might be possible. Therefore an arrangement has been suggested [2] consisting of continuous, orthogonal, intersecting electron (or X-ray), molecular and laser beams. Limited coherence of the electron beam ensures that no interference occurs between the wavefields scattered by different molecules within the electron beam. The diffraction pattern is a sum of the intensities of the identical patterns from the many hydrated molecules within the beam at any one time. The two-dimensional electron diffraction pattern accumulates continuously at the detector for a fixed laser and molecular orientation before being read out. Repeating this process for many orientations would allow tomographic reconstruction of the molecule. An electron diffraction camera with a water droplet source, a polarized laser beam and a LaB_6 electron gun is currently under development. Initially we use micron size water droplets and dope them with large particles like TMV, since they are easier to align. Preliminary results with this instrument will be presented.

[1] Spence J., Doak T., *Phys. Rev. Lett.*, 2004, **92**, 198102–198104. [2] Spence J.C.H., Schmidt K., et.al., *Acta Cryst.*, 2005, **A61**, 237–245.

Keywords: electron diffraction, protein structure determination, image reconstruction

MS69.28.2

Acta Cryst. (2005). A**61**, C88-C89

Methods Development and Software Engineering for 2D Electron Crystallography

Ansgar Philippsen[a], Andreas Schenk, Giani Signorell, Wanda Kukulski, Andreas Engel, [a]*Maurice Müller Institute for Structural Biology, Biozentrum, University of Basel, Switzerland.* E-mail: ansgar.philippsen@unibas.ch

Electron crystallography of 2D crystals (2D-EX) of membrane proteins has allowed atomic models of these proteins to be build (1,2). Several advantages of this method over 3D x-ray crystallography can be identified, such as preserving the protein in a more native state or imaging of the crystal with direct amplitude and phase retrieval. Nevertheless, this method has not yet matured to the point of routine use. We pursue the goal to establish 2D-EX membrane protein crystals as a complementary method (next to x-ray crystallography and structural NMR) for resolving atomic resolution structures of biological macromolecules. To this end, we are in the process of implementing and refining the methods utilized by the pioneers of the field (1,2), as well as following novel methodological and algorithmic approaches. In parallel, we are developing an image processing library and toolkit (3), taylored to the specific requirements of these methods.

[1] Henderson R., Baldwin J.M., Ceska T.A., Zemlin F., Beckmann E., Downing K.H., *J. Mol. Biol.*, 1990, **213**, 899. [2] Murata K., Mitsuoka K., Hirai T., Walz T., Agre P., Heymann J.B., Engel A., Fujiyoshi Y., *Nature*, 2000, **407**, 599. [3] Philippsen A., Schenk A.D., Stahlberg H., Engel A., *J.*