

experimental evidence that xenon reacts with SiO<sub>2</sub> at high pressures and temperatures [1].

The evolutionary algorithm USPEX [2,3], used here for predicting new stable structures, searches for the structure with the lowest free energy at the given P-T conditions and is capable of predicting the stable structure of a compound knowing just the chemical composition. The underlying *ab initio* structure relaxations were performed using density functional theory (DFT) with the generalized gradient approximation (GGA) together with the all-electron projector augmented wave (PAW) method, as implemented in the VASP [4] code.

Using the *ab initio* evolutionary algorithm USPEX, we investigated the stability of Xe-O compounds at high pressures. Present results clearly show that Xe loses its chemical inertness under pressure and that charge transfer plays an essential role in chemical bonding in Xe compounds and stability of these compounds is largely determined by electronegativity differences.

XeO (space group *Pbcm*) and XeO<sub>2</sub> (space group *Pnma*) have been found to be thermodynamically stable at pressures above 89 GPa and 102 GPa, respectively, with xenon adopting increasingly more oxidized states on increasing pressure. Extending our calculations to the Xe-Si-O system, we found no stable xenon silicates at pressures relevant to the Earth's mantle (<136 GPa). However, energetically favoured structural analoga to the xenon oxides were found in the silicon oxides, pointing to a preferred Xe coordination, which could be found in a possible stable xenon silicate.

[1] Sanloup C., Schmidt B.C., Perez E.M.C., Jambon A., Gregoryanz E., Mezouar M., *Science*, **2005**, 310, 1174. [2] Oganov A.R., Glass C.W., *Journal of Chemical Physics*, **2006**, 124, 244704. [3] Glass C.W., Oganov A.R., Hansen N., *Computer Physics Communications*, **2006**, 175, 713. [4] Kresse G., Furthmüller J., *Physical Review B*, **1996**, 54, 11169.

**Keywords:** *ab-initio* calculations; crystal structure prediction; xenon oxides

#### FA5-MS07-P04

**Microfocus X-ray Sources for Short Wavelength Radiation.** Joerg Wiesmann<sup>a</sup>, Joergen Graf<sup>b</sup>, Bernd Hasse<sup>a</sup>, Carsten Michaelsen<sup>a</sup>. <sup>a</sup>*Incoatec GmbH, Geesthacht, Germany.*

E-mail: [wiesmann@incoatec.de](mailto:wiesmann@incoatec.de)

Combining synthetic multilayer mirrors with microfocus X-ray sources (rotating or stationary target) has, over the past years, become standard in home lab X-ray sources for single crystal diffraction and for certain applications in powder diffraction [1]. In contrast to multilayer mirrors for Cu sources, the maximum angles of incidence at which a multilayer mirror reflects higher energy radiation, such as Mo-K<sub>α</sub> or Ag-K<sub>α</sub> radiation, are significantly smaller than for Cu radiation. With today's deposition technology, however, high quality multilayer mirrors can be produced which have a small *d*-spacing and reflect higher energy radiation at larger angles of incidence [2, 3]. Together with the latest developments of microfocus sealed tubes, this makes way for new high-performance low-power X-ray sources for

shorter wavelengths.

We will present selected results on the use of microfocusing sealed tube X-ray sources with high-performance focusing multilayer mirrors for Mo-K<sub>α</sub> and Ag-K<sub>α</sub> radiation applied in small molecule and high-pressure crystallography.

[1] Wiesmann J., Hoffmann C., Graf J., Michaelsen C., **2007**, New Possibilities for X-ray Diffractometry, *Physics Meets Industry* (Eds. J. Gegner, F. Haider), p. 13 - 20, Expert Verlag, Renningen. [2] Michaelsen C., Wiesmann J., Hoffmann C., Oehr A., Storm A.B., Seijbel L.J., **2004**, *Proc. SPIE* 5193, 211. [3] Schuster M., Göbel H., Brügemann L., Bahr D., Burgázy F., Michaelsen C., Störmer M., Ricardo P., Dietsch R., Holz T., Mai H., **1999**, *Proc. SPIE* 3767, 183.

**Keywords:** X-ray optics; new XRD technology; high-pressure crystallography

#### FA5-MS07-P05

**Core Ionization in Compressed Alkali and Alkali-Earth Metals.** Valentina Degtyareva. *Institute of Solid State Physics, Russian Academy of Science, Chernogolovka, Russia.*

E-mail: [degtyar@issp.ac.ru](mailto:degtyar@issp.ac.ru)

Under compression, simple s-bonded alkali and alkali-earth metals pass through the sequence of phases characterized by lowering in symmetry, coordination number and packing density [1,2]. Structural transformations in these metals are controlled by the combined effects of electrostatic (Madelung) and electronic (band-structure) contributions to the crystal energy. The latter term increases with pressure yielding low-symmetry complex structures, such as cI16 in Li and Na, Rb-oC52 and Cs-oC84. Stability of these structures can be supported by a Hume-Rothery argument when new diffraction plains appear close to the Fermi level [3].

Upon further compression heavy alkalis Cs and Rb form a very open structure tI4 with coordination number 4+4 and packing density ~0.56. Considering the Brillouin zone configuration with respect to the Fermi sphere one can conclude that the Hume-Rothery mechanism is effective if the number of valence electrons increases from 1 up to 2 and higher values implying the transition of the outer core electrons into the valence band.

Similar changes in the valence state are expected for compressed Na at the transition from cI16 to oP8 at pressures above 117 GPa [2]. Observations of the simple cubic structure in Ca (above 32 GPa) and the beta-tin structure in Sr (above 25 GPa) imply the increase in the number of valence electrons resulting from the core ionization [3].

[1] McMahon M.I. and Nelves R.J., *Chem. Soc. Rev.* **2006**, 35, 943. [2] Gregoryanz E. et al., *Science* **2008**, 320, 1054. [3] Degtyareva V.F., *Phys. Usp.* 2006, 49, 369.

**Keywords:** high pressure; crystal structures; alkali metals