s6.m2.o1 High-Pressure powder crystallography using synchrotron- and neutron-radiation. M. Kunz, *Laboratory of Crystallofraphy, ETH Zürich, CH-8092Zürich*.
Keywords: extreme conditions.

The exploration of material under conditions of high pressure and high temperature is a frontier challenge in crystallography. Diffraction techniques using X-rays and neutrons are most useful methods to obtain information on the structure of condensed matter also under non-ambient conditions. Difficulties to preserve a single crystal at extreme P and T as well as geometric constraints of the sometimes sophisticated sample-environments make powder-diffraction the method of choice to extract diffracted intensities from a sample subject to extreme pressure and temperature. Inherent problems such as small sample volumes, additional background from pressure cells, non-hydrostatic stress and limited accessibility of reciprocal space contribute to a general deterioration of the quality of data when compared to ambient conditions. Powder crystallography at extreme conditions thus relies critically on a high flux of the radiation source, sensitive detectors and versatile data analysis software.

Although the P-T regime accessible with laser heated diamond anvil cells (as they are used in combination with synchrotron X-rays) and large volume cells (as they are necessary for neutron high-pressure work) are very different, the complementarity of neutrons and X-rays is highly beneficial when solving crystallographic problems at high-pressure and temperature. It therefore comes as no surprise that in both domains (synchrotron X-ray- and neutron-diffraction) large progress with respect to experimentation at extreme conditions have been achieved in recent years.

The combination of diamond anvil cells, laser-heating and synchrotron radiation allows for monochromatic *in situ* experiments up to the megabar range at temperatures of several 1000 K. Rietveld refinements have been successfully applied to such data[1]. On the neutron side, most high-pressure work has so far been done in combination with TOF techniques[2,3]. Recent developments, however, show the potential of angle dispersive neutron diffraction up to pressures of 50 GPa [4].

This talk will review the state of the art in powder crystallography at extreme conditions using synchrotron and neutron radiation. Emphasis will be given on new developments and possible future trends to overcome inherent problems of such experiments.

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[4] Goncharenkov et al.: "Focusing Neutrons to study small samples" Physica B (1997), 234 1047 - 1049.

s6.m2.o2 The chemical bond under high pressure and at high temperature: semiconductor to metal transition in covalent systems. J.-P. Gaspard and J.-Y. Raty. *Condensed Matter Physics Physics department - B5 University of Liege 4000 SART-TILMAN (Belgium) jp.gaspard@ulg.ac.be*
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In this review we first study of a generic elemental semiconductor: selenium at high pressure and high temperature. We then give a systematic review of a series of elemental and compound semiconductors ranging from zero dimensional to three dimensional systems.

The study integrates experimental results obtained by X-Ray scattering and EXAFS in different high pressure cells, as well as neutron diffraction experiments in the liquid phase.

A theoretical semi-empirical models is proposed: it allows to systematise the pressure dependence of the interatomic distances, the bulk modulus, the transition pressure and the nature of the semiconductor-metal transition in covalent systems. Total energy calculations are shown and the importance of the repulsive potential is stressed. Elemental semiconductors (As, Se, Br,..) are considered as well as binary compounds (GaSb, InSb, HgTe,..). Negative pressures are also considered in the case of alkali atoms in chlathrates.