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High-pressure melting of silicon. Innokenty Kantora,b, Vitaly Prakapenkaa. *GSECARS, Advanced Photon Source, Argonne, USA. bESRF, Grenoble, France. E-mail: kantor@cars.uchicago.edu

Silicon is one of the most intensively used chemical elements in the modern technology. The vast majority of semiconductive electronics, CCD chips, solar batteries, etc. is based on pure or doped silicon. Silicon is also considered as a possible light element in the Earth’s core, and therefore its high-pressure and temperature properties are also important for geosciences.

There are seven known silicon phases at high pressure [1,2]. Accurate measurements of Si phase diagram including melting curve were performed at a large-volume multianvil press, and are limited to pressures of about 15 GPa [3].

There are two main experimental challenges of doing laser heating melting experiments in a diamond anvil cell. First is the detection of melting: Si is a relatively weak X-ray scatterer and it is difficult to observe diffraction from a melt liquid. Second difficulty is the accurate temperature determination. At low pressures Si melts at temperatures around 1000 K, which is below the limit of conventional spectrographic temperature measurements.

With the advanced laser-heating facility at 13IDD and a high brightness monochromatic X-ray beam with fast CCD area detector it was possible to map Si phase diagram and to determine melting curve of silicon even at lowest pressures.


Keywords: high-pressure diffraction, melting, silicon

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Single crystal diffraction at Earth’s mantle conditions. Marco Merlini, Università degli Studi di Milano, Dipartimento di Scienze della Terra, Milano, Italy. E-mail: marco.merlini@unimi.it

Recent improvements at synchrotron beamlines and on Diamond Anvil Cells techniques allow single crystal diffraction experiments at non ambient conditions on very small crystals, one order of magnitude smaller compared to samples routinely investigated on conventional laboratory sources. Three examples concerning high pressure single crystal diffractions at Earth’s Mantle conditions will be illustrated and discussed: structural determination of CaFe2O4 crystal diffractions at Earth’s Mantle conditions will be illustrated and discussed: structural determination of CaFe2O4 and CaCO3 across electron Fe2+ and Fe3+ spin transition (around 50 GPa) and elasticity and phase transitions of CaFeO3.5 defective brownmillerite/perovskite at lower mantle conditions.

Keywords: single crystal, high pressure Earth’s lower mantle

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High-Pressure Synthesis of Rare Earth Metal Polychalcogenides. Thomas Doerta, Carola J. Müllera,b, Ulrich Schwarza, Peer Schmidt. *Department of Chemistry and Food Chemistry, TU Dresden, Germany. bMax Planck Institute of Chemical Physics of Solids, Dresden, Germany. E-mail: thomas.doert@chemie.tu-dresden.de

The structural chemistry of the polychalcogenides of the trivalent rare earth metals LnX2.8 (Ln = Y, La – Nd, Sm, Gd – Lu; Lu: X = S, Se, Te; 0 ≤ δ < 0.3) is characterized by a multiplicity of compounds which exhibit closely related crystal structures with slightly different compositions: LnX2.0, LnX1.9, LnX1.875, and LnX1.8. Structurally, all compounds can be regarded as superstructures of the ZrS2 type containing puckered [LnX]2 double sheets and planar [X1.8] layers. Depending on δ, the anionic layers contain X2– dimers, X+ anions and vacancies. Thermoanalytical and tensimetric studies reveal that polysulfides and polyselenides LnX2.8 generally decompose at elevated temperatures by a stepwise release of molecular chalcogen X2 to form the adjacent metal richer phase according to the reaction

20 LnX2.8(s) → 20 LnX1.8(s) + X2(g), e. g.

The decomposition process stops as soon as the sesqui-chalcogenide Ln2X3 is finally reached. Polychalcogenides of the smaller rare-earth metals are known to have higher decomposition pressures. For this reason all attempts to synthesize stoichiometric disulfides or diselenides of those metals under ambient pressure conditions failed up to now. In a series of experiments we synthesised rare earth metal polychalcogenides under high pressure conditions to directly counteract the decomposition pressure. Single phase powder samples of several LnX2.0 and LnX1.8 phases were prepared at pressures up to p = 8 GPa and temperatures up to T = 1450° C [1,2]. Under optimised reaction conditions it was also possible to obtain twinned crystals of GdS2, TbS2, ErS2 and TmS2, suitable for X-ray structure determination. The disulfides adopt the monoclinic α-LaS2 structure [3] (space group P21/a), TmS2 crystallises in the CeS2 type [4] in space group P42/n. All investigated LnX2.8 phases are semiconductors and contain Ln2+.

Keywords: Polychalcogenides, rare earth, high pressure