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Raman spectroscopy and X-ray diffraction *in situ* characterization of phase transitions in cristobalite under high pressure

V. B. Prokopenko[a,*], L. S. Dubrovinsky[a], V. Dmitriev[b], H.-P. Weber[b]

[a] Department of Earth Science, Uppsala University, S-752 36 Uppsala, Sweden
[b] European Synchrotron Radiation Facility, Grenoble 38043, France
[*] Corresponding author. *E-mail address:* vitali.prokopenko@geo.uu.se

We have studied *in situ* the structure and optical properties of cristobalite at pressures up to 61 GPa by means of micro-Raman spectroscopy and X-ray powder diffraction. The α-cristobalite phase of SiO_2 was formed after annealing of silica sol-gel glass at 1500^0C for 15 minutes. For generation of high-pressure a Mao-Bell and membrane type diamond anvil cells were used. On pressure increase four polymorphs were found: C-I has initial structure of α-cristobalite up to 6 GPa, C-II in the pressure range 0.2 – 14GPa, C-III from 14 to 35, C-IV above 35 GPa, and no new phase was observed up to 61 GPa. The high-pressure phase C-IV is crystalline and quenchable. The monoclinically distorted α-PbO_2-type structure provides the best fit of X-ray pattern of recovered C-IV phase.

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Experimental and Theoretical Identification of New High-Pressure TiO_2 Polymorph

Natalia A. Dubrovinskaia[*], Leonid S. Dubrovinsky[*], Rajeev Ahuja[§], Vitaly B. Prokopenko[*], V. Dmitriev[£], H.-P. Weber[£], J. M. Osorio-Guillen[§], Börje Johansson[§]

** Bayerisches Geoinstitut, Universität Bayreuth, D-95440 Bayreuth, Germany*

§ Department of Physics, Uppsala University, S-751 21 Uppsala, Sweden

[£] SNBL, European Synchrotron Radiation Facility, Grenoble 38043, France

Our combined theoretical and experimental investigations have led to the discovery of a new polymorph of titanium dioxide, where titanium is seven-coordinated to oxygen in the orthorhombic OI (*Pbca*) structure. The zero-pressure bulk modulus of the new phase measured in the pressure range 19 to 36 GPa is 318(3) GPa. We demonstrate that the group IVa dioxides (TiO_2, ZrO_2, HfO_2) on compression at ambient temperature all follow the common path: Rutile –> α-PbO_2-type -> baddeleyite-type (MI) -> orthorhombic OI (*Pbca*) structure -> cotunnite-type (OII).

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Structure of Metallic and Magnetic High-Pressure Fe_3O_4 Polymorph: Experimental and Theoretical Study

L. S. Dubrovinsky[*], N. A. Dubrovinskaia[*], C. McCammon[*], G. Kh. Rozenberg[%], R. Ahuja[§], J. M. Osorio-Guillen[§], V. Dmitriev[£], H.-P. Weber[£], T. Le Bihan[#], B. Johansson[§]

**Bayerisches Geoinstitut, Universität Bayreuth, D-95440 Bayreuth, Germany*

[%] School of Physics and Astronomy, Tel Aviv University, Ramat Aviv, 69978 Tel Aviv, Israel
§ Department of Physics, Uppsala University, S-751 21 Uppsala, Sweden

[£] SNBL, European Synchrotron Radiation Facility, Grenoble 38043, France

[#] European Synchrotron Radiation Facility, Grenoble 38043, France

Studies of the nature of the high-pressure polymorph of magnetite, the oldest known magnetic material, have a long and controversial history. Using electrically- and laser-heated diamond anvil cells at pressures above 40 GPa we synthesized pure high-pressure Fe_3O_4 phase (h-Fe_3O_4) and performed an *in situ* structural refinement. In good agreement with our *ab initio* calculations we found that h-Fe_3O_4 adopts the $CaTi_2O_4$-type structure (space group *Bbmm*). Electrical resistivity and Mössbauer spectroscopy measurements show that h-Fe_3O_4 is metallic and magnetic up to at least 70 GPa. The magnetic properties are associated with one of the structural positions presumably occupied by mostly Fe^{2+} ions.