

FA2-MS17-P01

High pressure effects on the crystal and magnetic structure of $\text{Pr}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$. Deleg Sangaa^a, Denis P. Kozlenko^a, Sergey E. Kichanov^a, Tuan A. Tran^a, Zdenek Jiráček^b, Boris N. Savenko^a. ^aFrank Laboratory of Neutron Physics, JINR, 141980 Dubna Moscow Reg., Russia. ^bInstitute of Physics, Academy of Sciences, 16253 Prague, Czech Republic.
E-mail: sangaa@nf.jinr.ru

A crystal and magnetic structure of manganite $\text{Pr}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ has been studied by means of powder neutron diffraction at pressures up to 5 GPa in the temperature range 10–300 K. Under high pressure, a suppression of the initial pseudo-CE type antiferromagnetic (AFM) state and an appearance of A-type AFM state was observed. An anisotropic compression of the lattice was found which leads to the apical compression of MnO_6 octahedra. Possible mechanisms of the observed magnetic phase transition are discussed.

Keywords: Pressure; Magnetic Structure; Manganites

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High pressure structural studies of selected dicarbides. I. Efthimiopoulos^a, G. V. Vajenine^{a,b}, E. Stavrou^a, K. Syassen^a, St. Liebig^c, U. Ruschewitz^c, M. Hanfland^d. ^aMPI-FKF, Stuttgart, Germany. ^bInstitut für Anorganische Chemie, Universität Stuttgart, Germany. ^cDepartment für Chemie, Universität zu Köln, Germany. ^dESRF, Grenoble, France.
E-mail: ilias@fkf.mpg.de

Carbides of electropositive metals have attracted attention due to their physical properties such as superconductivity in layered MC_6 carbides with $M = \text{Y}$ or Ca [1]. The MC_6 compounds are formed by metal atom intercalation into graphite. Carbides with the MC_2 composition, featuring isolated C_2 dumbbells, have been characterized for all alkaline-earth and most rare-earth metals. For divalent metals these dicarbides are insulators or semiconductors. They can be viewed as acetylides featuring a triple carbon-carbon bond in the C_2^{2-} units. Interestingly, different valence electron counts might also lead to superconductivity such as in YC_2 [2]. Dicarbides of alkaline-earth metals crystallize with NaCl-related structures at ambient pressure. They are interesting candidates for in-situ high-pressure structural and spectroscopic investigations. On the one hand, changes in the local coordination in the course of structural phase transitions are of interest. On the other hand, possible polymerization of the C_2 dumbbells might lead to extended carbon networks. We have investigated the structural and vibrational properties of BaC_2 and CaC_2 under pressure by means of synchrotron-based X-ray diffraction and Raman spectroscopy. The ambient-pressure tetragonal $I4/mmm$ phase of CaC_2 [3] was found to be stable up to ~30 GPa, while the monoclinic C2/c phase fully converts into the tetragonal one below 7 GPa. When pressure exceeds 30 GPa, irreversible amorphization is observed, accompanied by a loss of the C_2 Raman signal. In contrast, the ambient-pressure tetragonal $I4/mmm$ phase of BaC_2 [4] undergoes a reversible phase transition at 4 GPa, accompanied by an increase of local coordination numbers. Similar to CaC_2 , BaC_2 becomes amorphous above 30 GPa. Simulations of the phase stability of CaC_2 and BaC_2 by first-principles calculations will be reported.

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Metastable Bi_2O_3 Polymorphs obtained by High Pressure and High Temperature. T. Locherer^a, S. Ghedia^a, A. Senyshyn^{b,c}, D. L. V. K. Prasad^a, R. Dinnebier^a, M. Jansen^a. ^aMax Planck Institute for Solid State Research, Stuttgart, Germany. ^bInst. For Materials Science, TU Darmstadt, Germany. ^cFRM II, Garching, Germany.
E-mail: t.locherer@fkf.mpg.de

Although being well known for the high ionic conductivity of its high temperature modifications, only little is known about the high pressure behavior of Bi_2O_3 . Previous reports contradict each other to a certain degree and do not present structures of high pressure modifications [1], [2]. Using a large volume multi anvil type device we were able to identify two new metastable (quenched to ambient conditions) polymorphs of Bi_2O_3 by means of X-ray and neutron powder diffraction. Structural analysis shows that in one of these modifications Bi_2O_3 crystallizes in an entirely new structure type within the non centrosymmetric space group $P31c$. The structure determining lone pairs for $\text{Bi}^{(III)}$ compounds are less pronounced on the $2b$ site and exhibit a highly polar orientation. These structural properties are giving raise to the assumption that the high pressure phase of Bi_2O_3 is a potential ferroelectric. Upon annealing it relaxes to a second new modification at about 106 °C, before at about 310 °C the transformation towards the stable ambient α -modification is completed. This “relaxed” phase can be considered as an intermediate polymorph similar to the ambient. In contrast to the former it exhibits a two dimensional channel network with the lone electron pairs pointing into these channels. A weak ionic conduction was determined for this modification.

[1] C. Chouinard, S. Desgreniers, *Solid State Commun.* 113 (2000) 125–129. [2] T. Atou *et al.*, *Mater. Res. Bull.* 33 No. 2 (1998) 289–292.

Keywords: High Pressure Phase Transformations, Lone Pairs, Neutron and X-ray diffraction

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Texture determination of ferroelectrics from *in situ* X-ray diffraction. Manuel Hinterstein^a, Michael Knapp^b, Hartmut Fuess^c, Helmut Ehrenberg^b. ^aComplex Materials, IFW Dresden, D-01069 Dresden, Germany. ^bCELLS, P.O.B 68, 08193 Barcelona, Spain. ^cMaterials Science, Technical University Darmstadt, Germany.
E-mail: manuel.hinterstein@desy.de

Piezoelectric ceramics such as lead zirconate titanate (PZT) or bismuth sodium titanate (BNT) with perovskite structure can be found in a multitude of applications. Most of these applications require electric poling, i.e. there must be a