

**MS18.01.05 HIGH PRESSURE PHASE TRANSITIONS OF RARE-EARTH GALLIDES REGa<sub>2</sub> (RE = Tm, Er, Ho).** S. Bräuninger, U. Schwarz, Yu. Grin and K. Syassen. MPI für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany.

We have investigated pressure induced structural changes of the rare-earth gallides REGa<sub>2</sub> (RE = Tm, Er, Ho) by means of x-ray powder diffraction using diamond anvil cell techniques. At ambient pressure ErGa<sub>2</sub> and HoGa<sub>2</sub> crystallize in the AlB<sub>2</sub>-type structure (*P6/mmm*) consisting of six-membered planar Gallium layers forming hexagonal prisms centered by the RE atoms. A common feature of all AlB<sub>2</sub>-type compounds REGa<sub>2</sub> is an *c/a* ratio close to the ideal value of 1.07 for touching spheres. ErGa<sub>2</sub> undergoes a discontinuous transition to the KHg<sub>2</sub>-type structure (*Imma*) near 6 GPa. The interlayer Ga-Ga distance 2.788(5) Å (7.6 GPa) is close to the Ga-Ga distance in TmGa<sub>2</sub> which crystallizes in this structure type at ambient pressure. In the KHg<sub>2</sub>-type the Ga atoms form six-membered rings in chair conformation. The layers are connected by Ga-Ga bonds along the crystallographic *a*-axis thus forming a three dimensional covalent gallium network of distorted tetrahedra with the RE atoms occupying the voids. ErGa<sub>2</sub> and TmGa<sub>2</sub> transform into the UHg<sub>2</sub>-type structure at 24 and 22 GPa respectively. The UHg<sub>2</sub>-type is a branch of the AlB<sub>2</sub>-type having a *c/a* ratio between 0.59 and 0.87. The pressure induced change of hybridization in these compounds results in a transition of a three-dimensional covalent network (KHg<sub>2</sub>) to a layered gallium partial structure (UHg<sub>2</sub>). The breaking of the interlayer Ga-Ga bonds was reproduced by LMTO calculations of the electron density and localization. A similar behavior is observed for HoGa<sub>2</sub>. However in this case a direct transition from the AlB<sub>2</sub>- to the UHg<sub>2</sub>-type takes place at about 5 GPa.

**MS18.01.06 NEUTRON DIFFRACTION STUDIES OF THE METALLIZATION PROCESS IN RNiO<sub>3</sub> PEROVSKITES (R = RARE EARTH).** M. Medarde<sup>1</sup>, J. Mesot<sup>1</sup>, S. Rosenkranz<sup>1</sup>, P. Radaelli<sup>3</sup>, W. Marshall<sup>4</sup>, S. Klotz<sup>5</sup>, J. S. Loveday<sup>4</sup>, G. Hamel<sup>5</sup>, S. Hull<sup>6</sup>. <sup>1</sup>Laboratory for Neutron Scattering, ETH&PSI, 5232 Villigen PSI, Switzerland; <sup>2</sup>Laboratoire des Fluorures, Université du Maine, Avenue Olivier Messiaen, 72017 Le Mans CEDEX, France; <sup>3</sup>Institut Laue Langevin, B.P. 156, 38042 Grenoble Cedex 9, France; <sup>4</sup>University of Edinburgh, Mayfield Road, Edinburgh, EH9 3JZ, U.K.; <sup>5</sup>University Paris VI, 4 pl. Jussieu, 75252 Paris Cedex 5, France; <sup>6</sup>Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX11 0QX, U.K.

RNiO<sub>3</sub> perovskites (R = rare earth different of La) show a very sharp metal-insulator transition /I/ at a temperature TM-I which increases by decreasing the size of the R ion (TM-I = 130, 200, 400 and 420 K for R = Pr, Nd, Sm and Eu, respectively). By applying an external pressure P, TM-I decreases at a constant rate (R-independent) of about -4 K/kbar. In order to investigate the structural changes associated to the metallization of the system, several neutron diffraction experiments have been performed at high pressure (up to 80 kbar) both at continuous and spallation neutron sources. The results indicate that, in contrast to the behavior observed in other perovskite compounds displaying the same space group (Pbnm) /2/, /3/, the distortion of the structure decreases with P /4/. The reasons for this unusual behavior are presented and the implications for the metallization mechanism discussed.

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**MS18.01.07 HIGH-PRESSURE STRUCTURAL STUDIES OF LANTHANIDES.** M.I. McMahon and R.J. Nelmes. Department of Physics and Astronomy, The University of Edinburgh, Edinburgh, EH9 3JZ, U.K.

The high-pressure behaviour of the elemental lanthanides still continues to attract considerable attention. Under pressure, the regular tri-valent lanthanides exhibit a series of phase transitions to simple close-packed structures, before undergoing further transitions to the so-called 'distorted-fcc' phase, and then to still more complex structures. The two di-valent lanthanides, Eu and Yb, however, exhibit different behaviour, as does Ce. In recent years, diffraction studies utilising improved experimental techniques have re-examined many of the complex high-pressure structures observed in all these systems, and have resolved many of the outstanding structural problems. Such studies have also cast new light on the physical basis of the observed behaviour. These recent advances will be reviewed, and new structural studies of Ce, Pr and Sm made at SRS Daresbury using angle-dispersive techniques and an image-plate area detector will be presented.

**MS18.01.08 HIGH-PRESSURE STUDIES OF ELEMENTAL METALS.** Kenichi Takemura, National Institute for Research in Inorganic Materials, Namiki 1-1, Tsukuba, Ibaraki 305, JAPAN

Most of the elemental metals have simple structures (bcc, fcc, and hcp) at atmospheric pressure. At high pressures, however, some metals exhibit structural phase transitions into unique low-symmetry crystal structures. One of the reasons for that is a change in the bonding properties from nearly spherical to highly directional ones. The pressure-induced electronic transition plays an important role in stabilizing such low-symmetry structures. As examples I will review the changes in the crystal structures of Cs [1] and Ba [2] under high pressure. Other unique crystal structures will also be presented including the singularity in the hcp structure recently found for Zn [3] and Cd [4].

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**MS18.01.09 CRYSTAL STRUCTURES OF ALKALI-METAL - TRANSITION METAL COMPOUNDS SYNTHESIZED UNDER PRESSURE.** J. V. Badding, L. J. Parker, T. Atou, Department of Chemistry, Pennsylvania State University, University Park, PA 16802.

We have developed techniques to investigate the formation of compounds between alkali metals and transition metals under pressure using a laser-heated diamond anvil cell. We report the synthesis of compounds in the potassium-silver and potassium-nickel systems. The high pressure syntheses, the diffraction techniques used to characterize the products, and their crystal chemistry will be described. These results demonstrate that the chemical behavior of the alkali metals under pressure is very different from that at ambient conditions. Synthesis of potassium-nickel compounds has implications for the hypothesis that potassium is incorporated into Earth's transition metal core.