

## MS19.P03

Acta Cryst. (2011) A67, C327

**Shock wave synthesis and properties of rocksalt-type of aluminium nitride**

Kevin Keller,<sup>a</sup> Thomas Schlothauer,<sup>a</sup> Marcus Schwarz,<sup>b</sup> Gerhard Heide,<sup>a</sup> Edwin Kroke,<sup>b</sup> <sup>a</sup>TU Mining Academy Freiberg, Institute for Mineralogy, Freiberg (Germany). <sup>b</sup>TU Mining Academy Freiberg, Institute for Inorganic Chemistry, Freiberg (Germany). E-mail: kevin.keller@mineral.tu-freiberg.de

Aluminium nitride is a ceramic material with a high thermal conductivity, a small thermal expansion coefficient and good mechanical properties. Moreover AlN is a wide-bandgap semiconductor ( $E_g = 6.2\text{eV}$ ) and therefore high potential substrate material for high-power electronic applications [1]. At pressure from 14-23GPa the wurtzitic aluminium nitride (wz) undergoes a phase transition to rocksalt structure (rs) at static experiments [2], [3], [4]. A sinterbody of wz-AlN/rs-AlN show high hardness (>4000HV), high electric resistance and a thermal conductivity up to 600W/mK [5]. Though the phase transition through shock waves were verified, shock experiments failed to quench the high-pressure phase so far [6].

Currently rs-AlN were successfully synthesized from AlN nanopowder with shock wave synthesis via flyer-plate method at the Freiberg High-Pressure-Research-Centre (FHP). A 80mm metal plate were accelerated by high explosive to several km/s striking a steel container with the pure AlN sample powder. To obtain good conditions a flat shock wave were produced with a special plane-wave-generator. The fine greyish powder (at the moment up to 2g per shot), which can be gathered from recovery container, shows up to 50% of the high-pressure AlN-phase. Caused by high oxygen content of the commercial AlN nanopowder, the synthesis product consist some percentage corundum and  $\gamma$ -AlON (up to 17%). At a given porosity of 1,68 at about 23GPa the highest yield can be achieved, while at higher pressures or major powder porosity, the post-shock-temperature is too high, so that the new high-pressure phase cannot be quenched and decomposes partly or complete to wz-AlN.

First experiments show good chemical resistance of rs-AlN to acids and bases and a thermal stability higher than 1100°C in air. Further analysis (FTIR, 27Al MAS-NMR, neutron diffraction and in-situ HT-XRD) are in progress.

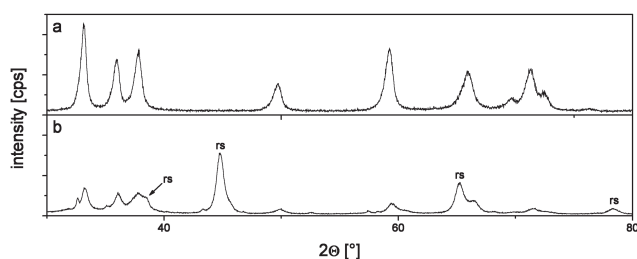


Fig 1: X-ray diffraction of (a) commercial nano-AlN-powder and (b) sample shocked at 22GPa with 50% rs-AlN yield.

[1] W. Werdecker, F. Aldinger, *Components, Hybrids, and Manufacturing Technology* **1984**, 7, 399-404. [2] I. Gorczyca, N.E. Christensen, P. Perlin, P. I. Grzegory, J. Jun, M. Bockowski, *Solid State Communications* **1991**, 79, 1033-1034. [3] M. Ueno, A. Onodera, O. Shimomura, K. Takemura, *Physical Review B* **1992**, 45, 10123-10126. [4] Q. Xia, H. Xia, A.L. Ruoff, *Journal of Applied Physics* **1993**, 73, 8198-8200. [5] H. Vollstadt, H. Recht, *Patent DD000000292903A5* **1991**. [6] K. Kondo, A. Sawaoka, K. Sato, M. Ando, *AIP Conference Proceedings* **1982**, 78, 325-329.

**Keywords:** aluminium nitride, shock wave synthesis, hard material

## MS19.P04

Acta Cryst. (2011) A67, C327

**New high-pressure-high-temperature forms in sesquioxides**

Sergey V. Ovsyannikov,<sup>a</sup> Xiang Wu,<sup>b</sup> Vladimir V. Shchennikov,<sup>c</sup> Alexander E. Karkin,<sup>c</sup> and Leonid Dubrovinsky,<sup>a</sup> <sup>a</sup>Bayerisches Geoinstitut, Universität Bayreuth, Bayreuth (Germany). <sup>b</sup>School of Earth and Space Sciences, Peking University, Beijing (China). <sup>c</sup>Institute of Metal Physics of Russian Academy of Sciences, Urals Division, Yekaterinburg (Russia). E-mail: sergey.ovsyannikov@uni-bayreuth.de

Sesquioxides,  $M_2O_3$  (where  $M$  – is a metal, like Al, Fe, Ti, Cr, Ga, etc.) (Fig.) are the focuses of interests of several fields, such as: geosciences, condensed matter physics and chemistry, industry and others. They show two trends in ambient crystal structure: oxides of metals of small periodic numbers  $Z$  prefer crystallization in a corundum structure, while those of metals of high periodic numbers prefer adopting in a cubic bixbyite lattice.

In this presentation we review new trends in high-pressure-high-temperature (HP-HT) studies in sesquioxides and report some of our new results on HP-HT preparation of novel forms of sesquioxides and examination of their properties. As an examples, we will display several important cases, some of which are listed below:

- (i) ‘Golden oxide’: Examination of electron band structure of the recently discovered golden  $Th_2S_3$ -type phase of  $Ti_2O_3$  [1], [2] by a set of experimental and theoretical methods.
- (ii) ‘Structural engineering’: fabrication of new structural forms in ‘mixed’ oxides, e.g. in  $(Ti_{1-x}M_x)_2O_3$  solutions by HP-HT synthesis.
- (iii) ‘Hidden phases’: the observation of new intermediate HP-HT phases in seemingly well-studied  $M_2O_3$  materials.
- (iv) ‘Composites’: not just mixtures of  $M_2O_3$ , but cases, like: ‘self-organization’, ordering, superstructuring and other puzzling processes in mixtures under HP-HT conditions; ‘hidden’ composite properties of a single structural phase of a single material prepared at HP-HT, etc.

[1] D. Nishio-Hamane, M. Katagiri, K. Niwa, A. Sano-Furukawa, T. Okada and T. Yagi, *High Pressure Res.* **2009**, 29, 379. [2] S. V. Ovsyannikov, X. Wu, V. V. Shchennikov, A. E. Karkin, N. Dubrovinskaya, G. Garbarino, and L. Dubrovinsky, *J. Phys.: Condens. Matter*, **2010**, 22, 375402.

**Keywords:** pressure, oxide, transition

## MS19.P05

Acta Cryst. (2011) A67, C327-C328

**Phase stability of boron relative to  $\beta$ -boron at high pressure and high temperature**

Jiaqian Qin, Tetsuo Irifune, Toru Shinmei, Hiroaki Ohfuji, Li Lei, *Geodynamics Research Center, Ehime University, (Japan)*. E-mail: jiaqianqin@gmail.com

Boron is one of the nonmetal elements that have been widely studied due to its complex polymorphism and fascinating chemical and physical properties. [1], [2] Boron’s three valences are too localized to make it metallic and insufficient in number to form a simple covalent bond. As a result, boron atoms form  $B_{12}$  icosahedra link together in a variety of ways. Until now, probably four of the reported boron phases correspond to the pure element. [1], [2]:  $\alpha$ -boron (rhombohedral, within a 12-atom unit cell),  $\beta$ -boron (high temperature form, rhombohedral, structure is not fully understood and consists of 105 or 108 atoms in