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

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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 γ -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.

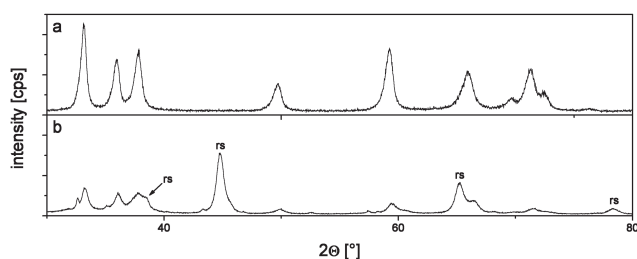


Fig 1: X-ray diffraction of (a) commercial nano-AlN-powder and (b) sample shocked at 22GPa with 50% rs-AlN yield.

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New high-pressure-high-temperature forms in sesquioxides

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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 $(\text{Ti}_{1-x}\text{M}_x)_2\text{O}_3$ 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.

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Phase stability of boron relative to β -boron at high pressure and high temperature

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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]: α -boron (rhombohedral, within a 12-atom unit cell), β -boron (high temperature form, rhombohedral, structure is not fully understood and consists of 105 or 108 atoms in