Contribution ID: **83** Type: **Oral contribution**

High-pressure synthesis of novel yttrium nitride, Y5N14, at 50 GPa

Tuesday 16 March 2021 10:35 (20 minutes)

Homonuclear dinitrogen anions are common intermediates in biological and organometallic synthetic chemistry, and play an important role in the processes of nitrogen reduction to ammonia. In extended solid-state compounds, nitrogen is typically present in the form of a nitride anion N3– and does not form catenated polyanions. However at high-pressure conditions MN2 dinitride compounds of alkali-earth metals (M = Ca, Sr, Ba), transition metals (M=Ti, Cr, Fe, Co, Ni, Cu, Ru, Rh, Pd, Re, Os, Ir, Pt) and rare earth metal (M = La) were obtained. In MN2 compounds, metals usually possess their common oxidation states, while the dinitrogen anion formally accommodates from 1 to 4 electrons. The degree of charge transfer from the metal to the nitrogen dimers significantly affects the properties of the materials (e.g. MN2 (M = Pt, Ir, Os, Ti) pernitrides with [N2]4– units are much less compressible than MN2 (M = Cr, Fe, Co, Ni, Ru, Rh) with [N2]3– units).
In this study yttrium and molecular nitrogen were compressed to 50 GPa and laser heated above 2000 K. Under these conditions, synchrotron single-crystal X-ray diffraction from multigrain samples revealed the formation of a new tetragonal yttrium nitride phase with the unusual Y5N14 composition (Fig. 1a). All nitrogen atoms form dimers, but strikingly there are three different types of nitrogen dimers in the structure with 1.24 Å, 1.28 Å and 1.36 Å nitrogen-nitrogen bond length (Fig. 1b). The bond length correlates with the multiplicity of the nitrogen-nitrogen bond and charge state of the nitrogen dimers. Our detailed analysis shows that there are six [N=N]2- dimers and one [N- ⊠N]3- dimer per Y5N14 formula unit, which corresponds to the typical Y3+ oxidation state for all yttrium atoms. Ab-initio calculations confirm that this structure is dynamically stable at such pressure.
Although [N2]2- and [N2]3- ions are known in the structures of other dinitrides, Y5N14 is the first example of the presence of two different types of charged nitrogen dimers in the same structure, which indicates more complex chemical processes of dense dinitrides formation under high pressure.

Fig. 1. a) Structure of the novel Y5N14 phase and b) different dinitrogen anions in the Y03 atom coordination environment.

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Session Classification: Inorganic crystal structures

Track Classification: Inorganic crystal structures