MS27 Minerals and Materials Under Extreme Conditions

MS27-05

Binary arsenic nitride synthesized from elements under pressure

K. Dziubek [1], M. Ceppatelli [2], D. Scelta [1], M. Serrano-Ruiz [3], M. Morana [4], V. Svitlyk [5], G. Garbarino [5], T. Poręba [5], M. Mezouar [5], M. Peruzzini [3], R. Bini [6]

[1]LENS - Sesto Fiorentino (Italy), [2]LENS, CNR-ICCOM - Sesto Fiorentino (Italy), [3]CNR-ICCOM - Sesto Fiorentino (Italy), [4]University of Pavia - Pavia (Italy), [5]ESRF - Grenoble (France), [6]LENS, University of Florence - Sesto Fiorentino (Italy)

Abstract

Synthetic nitride chemistry is a very rapidly developing field. Many nitrides and nitride-based heterostructures are promising materials that can find application as superhard compounds, wide-bandgap semiconductors *etc*. Applying different high pressure-high temperature techniques facilitates nitridation and is the key to the synthesis of novel phases directly from elements.

Both nitrogen and arsenic belong to group 15 of the periodic table, although they exhibit completely different physical and chemical properties. At normal conditions nitrogen consists of very stable (945 $kJmol^{-1}$) N≡N molecules, while the ground state of arsenic, so-called grey modification, is a solid-state structure consisting of extended layers. The direct chemical reaction between arsenic and nitrogen has not been reported. Indeed, except for the $As(N_3)_3$ and $As(N_3)_5$, the unstable and explosive molecular azides synthesized from the precursors, no binary compound of As and N has been revealed so far.

We report for the first time the high-pressure high-temperature synthesis of extended covalent AsN from elements at P > 25 GPa and T > 1400 K [1]. The cubic crystal structure (space group $P2_13$), in which each arsenic atom is single-bonded to three neighbouring nitrogen atoms and vice versa (Fig. 1), has been reported so far for only several binary compounds: yellow α-indium (I) chloride InCl, α-cubic tin (II) sulfide SnS, and intermetallic phases strontium aluminide SrAl and strontium gallide SrGa. The arrangement of atomic or ionic units in these crystals resembles a severely distorted rocksalt structure, with a doubled lattice parameter. The new material was investigated also on compression and decompression, confirming its (meta)stability at room temperature in the pressure range of 10-50 GPa.

References

[1] Ceppatelli, M.; Scelta, D.; Serrano-Ruiz, M.; Dziubek, K.; Morana, M.; Svitlyk, V.; Garbarino, G.; Poręba, T.; Mezouar, M.; Peruzzini, M.; Bini, R. *Angew. Chem. Int. Ed. Engl.* **2022**, *61*, e202114191.