RESEARCH OF PHASE TRANSITIONS IN ALKALINE METAL PNICTIDES AT HIGH PRESSURE

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It is known, that at atmospheric pressure alkaline metal pnictides A_3B (A = Li, … Cs, B = N, … Bi) crystallize in three different structure types: hexagonal structure types AlB_2 and Na_3As, and cubic - Li_3Bi or NaTl. The last structural type is characteristic only of such compounds, as Cs_3Sb and Cs_3Bi [1], i.e. with a maximum atom radius of alkaline metal. At pressure less than 1.0 GPa and room temperature Li_3N (structural type AlB_2) undergoes polymorphic transformation in the denser structure Na_3As, is metastable in usual conditions [2], and at higher 8.0 GPa – can transformed in cubic structure [3]. The information about a behavior Li_3P, Na_3Sb and Na_3Bi at high pressure practically is absent.

The synthesis at high pressure was performed in a toroid type apparatus [4] at pressure up to 8 GPa and 1370-1870 K. Pressure and temperature value were estimated usual for "solid-phase" chambers by an indirect method - by preliminary calibration. The control an amount and structure of phases on all stages of synthesis have carried out by methods diffraction quenching after HPHT treatment samples (XRD analysis, Cu-K_α radiation), or in-site in a pressure range 10^{-4}-9.0 GPa in the diamond high-pressure chamber at room temperature [5].

There is shown, that the irreversible polymorphism is characteristic only for lithium antimonide. The cubic modification of lithium phosphide is obtained at high pressure and temperature (4 GPa, 400 K) [6], but this modification remains steady under usual conditions only within several hours.

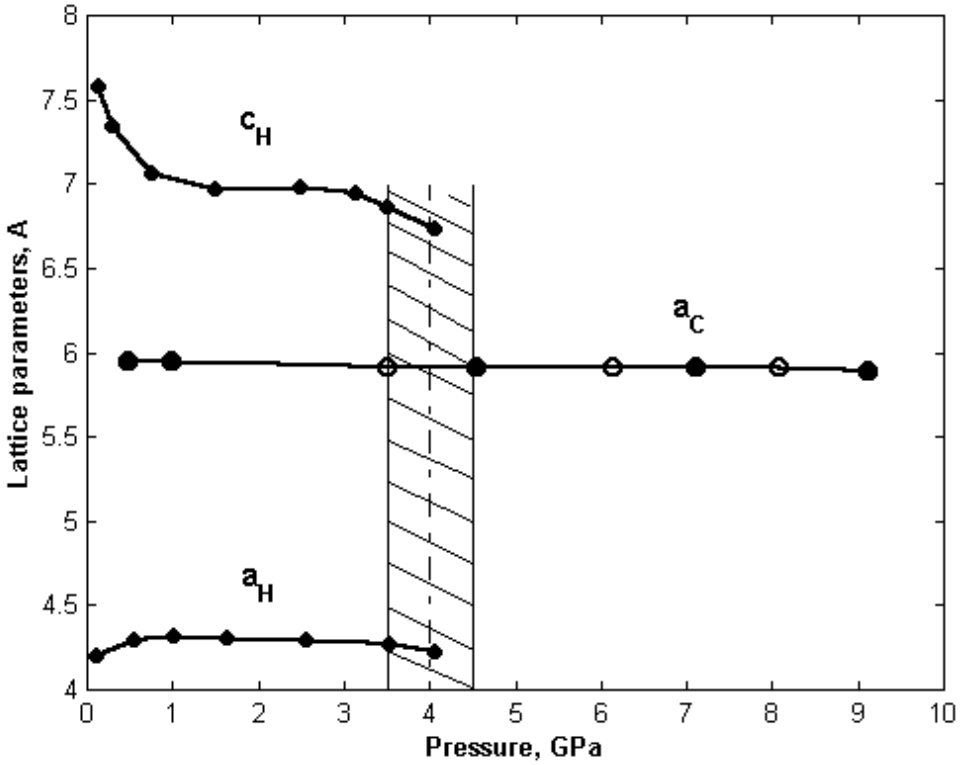

Fig 1. Dependence of lattice parameters for hexagonal (a_H, c_H) and cubic (a_C) structures from pressure. Dark circles- increasing pressure, open circles- decreasing pressure.

The modification of lattice parameters Li_3P under pressure in situ (some cycles "loading - reloading") is shown.

Sodium antimonide and sodium bismuthide undergoes converted phase transitions of a hexagonal structure in cubic one at pressure 2.3 and 0.75 GPa accordingly at room temperature, confirms data of

work [3].

The phases of high pressure of these compounds remained steady at high pressure only. The full reloading reduced in returning in initial hexagonal structure.

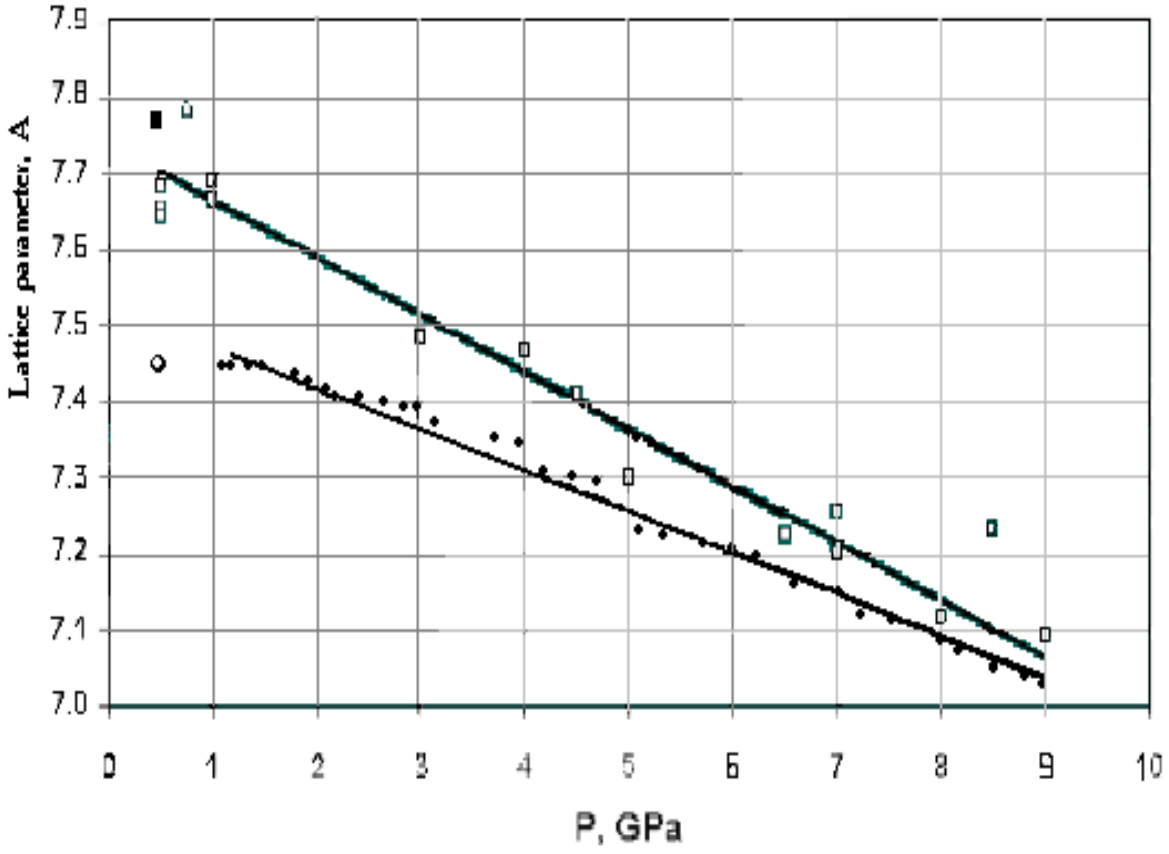

Fig 2. Dependence of lattice parameters Na_3Bi (□) and Na_3Sb (•) from pressure.

It is shown (fig 2), that the parameter of a cubic lattice Na_3Sb varies less sharply on a comparison with a modification of lattice parameter Na_3Bi.

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