High pressure, high temperature crystallography of graphite intercalation compounds

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Carbon framework of graphite structure can host alkali metals between layers forming graphite intercalation compounds (GIC). In the case of GICs with multiple layers separated by metallic layer, one can imagine graphite-to diamond transformation in carbon framework, leading to “diamond intercalation compounds” (DIC). The design of such material(s) was the purpose of our work.

GIC with metals such as Li, Na and K form different compositions (and crystal structures) are produced by stacking along c-axis of metal (Me) and *n* carbon (A, B or C) layers. The *n* number indicate the stage of intercalation. Typically ordered compounds are obtained for $n = 1$ to 6 with various stacking sequences depending on metals: $n = 1$ for MeAMeB, $n = 2$ for MeABMeBAMeCA, $n = 3$ for MeABCMeBCAMeCAB, etc. Experiments show that both high pressure and high temperature leads to increasing *n*. We will discuss the structural features of GIC, the XRD, Raman and other structurally related data, as well as corresponding DIC structurally related to GIC. The pressure and temperature range of formation of DICs from GICs coincide with industrially accessible conditions, that allows considering them as new promising materials. We have also shown that powder XRD is a method o fchoice for study of such transformations.

Keywords: **carbon framework, graphite intercalation compounds, high pressure, design of advanced materials**