

HIGH-PRESSURED C₇₀ PHASES: MODELING AND DIFFRACTION ANALYSIS

L. Chernozatonskii^a, N. Serebrynaya^b

^a*Institute of Biochemical Physics of RAS, 119991 Moscow, Russia*

^b*Institute of Spectroscopy of RAS, 142190 Troitsk, Russia*

Polymeric fullerenes have attracted considerable interest due to their unique nanoscale networks and high hardness of their 3D polymer structures.

Here we present structure modelling of new polymeric forms of fullerite C₇₀ material, which have obtained during high pressure - high temperature treatment (V. Blank group, 1995-2002). The crystal structures have been studied by X-ray powder diffraction and molecular dynamic modelling with following profile analysis of diffraction patterns by using DICVOLV and Rietveld programs.

We have modelled precursor phase, which has been observed under lower pressure (up to 5 GPa, <700 K) and is very close to low temperature monoclinic up to phase discovered by D. Cox group (Chem.Phys. **178**, 1993, 599). Then fullerenes have reconstructed into polymer phases under high-pressure-temperature (≥9GPa, ~700 K) influence. We have obtained good conformity between theoretical model and experimental data of fullerene chain atomic structure (up to 9GPa, ~700 K). This phase differs from “zigzag” chain structure observed by A. Soldatov et al (Science **293**, 2001, 680). We have found that diffraction pattern of this monoclinic chain phase is close to that of a phase observed under pressure 5GPa (~700 K) by Y. Iwasa group (Appl. Phys. A **64**, 1997, 251).

Under higher (9.5-15 GPa, ≥700 K) pressure we have observed transformation of solid C₇₀ into superhard 3D polymer phase and supposedly into single wall nanotubes. We have modelled new tetragonal structure of 3D polymerized fullerite C₇₀ transformed from the chain phase. The mechanisms and scenario of such transformations of C₇₀ chains into (5,5) nanotubes are also considered using computer modelling.

This work was supported by INTAS (00-237), Program “Topical directions in condensed matter physics”.