Graphite-like BN-C solid solutions are promising precursors for the high-pressure synthesis of novel superhard phases in the B–C–N system. Recently phase transitions of turbostratic graphite-like BC$_2$N up to 30 GPa have been studied in a DAC using X-ray diffraction with synchrotron radiation [1]. With the aim of explaining the observed evolution of diffraction patterns under compression at room temperature, we have performed the Rietveld analysis of the experimental patterns and simulated diffraction patterns of layered finite-size B–C–N clusters with lattice defects of various types [2].

Our findings have shown that above 20 GPa a reversible diffusionless transformation of the initial turbostratic structure into disordered layered high-pressure phase takes place. The general mechanism of the process includes disordering in interlayer spacings, buckling of layers and abrupt change of interlayer spacings attributed to the formation of the disordered high-pressure phase consisting of close-packed buckled layers with a diamond-like structure (Figure).

References: