The effect of shear deformation on C–N structure under pressure up to 80 GPa

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We studied the effect of shear deformation upon graphitic (g) C_3N_4 under pressure of up to 80 GPa at room temperature. Samples of g-C_3N_4 are transformed from initial amorphous flakes into onion-like structures, in which the nitrogen content in the quenched samples decreases with increasing pressure (from 0.42 in the initial to 0.01 at 80 GPa). The concentration of the sp^2 bonds also decreases from 1 (the initial sample) to 0.62 with increasing pressure to 80 GPa. This transformation of the sample is due to the fact, that in the pressure range of 55–115 GPa, the equilibrium phase is not a diamond, but carbon onions cross-linked by sp^3-bonds, which are denser than diamonds. The results of our study show that the presence of nitrogen in sp^3 bonded structures at pressures higher than 55 GPa reduces the density and, accordingly, carbon structures without nitrogen become thermodynamically favorable.