

o.m7.o5 Single-crystal study of the polymer layer stacking in the high-pressure two-dimensional C₆₀ polymers. R. Moret, P. Launois, *Laboratoire de Physique des Solides, UMR CNRS 8502, Université Paris-Sud, 91405 Orsay, France*, T. Wågberg and B. Sundqvist, *Department of Experimental Physics, Umeå University, 90187 Umeå, Sweden*

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High-pressure high-temperature polymerisation of C₆₀ leads to a variety of new crystalline and amorphous phases which display interesting physical properties. The mechanism of formation and the stability of these phases are still poorly documented and understood. Up to about 8GPa and 800-900K, polymer phases are formed through covalent bonding of C₆₀ molecules (2+2 cyclo-addition). These phases had been characterised so far from studies performed on powders. We have obtained, for the first time, 1D and 2D polymers by high-pressure high-temperature treatments of pristine C₆₀ single crystals¹.

We report here on the study of a 2D polymer crystal treated at 700K and 2GPa². Crystalline order is preserved but the crystal splits into orientational variants. The analysis of x-ray diffraction and Raman spectroscopy data reveals that the polymer crystal is primarily tetragonal with some admixture of a rhombohedral phase. For the tetragonal phase, it is shown that successive polymer layers are rotated by 90° about the stacking axis, according to the P4₂/mmc space group symmetry. The structure of the rhombohedral phase is also clarified. These results are at variance with previous structural reports. On the other hand, they agree with some predictions based on lattice energy minimisation.

Using these results we analyse the intermolecular environments in the polymers to obtain some information on the role of the interlayer interactions in stabilising the observed polymer structures. The mechanism of formation of the C₆₀ polymers (dimers, chains, layers) and their transformations are also discussed.

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[2] R. Moret, P. Launois, T. Wågberg and B. Sundqvist, *European Phys. Journal B*, (2000), in press.