Behavior of Hexagonal Close Packed Metastable Phase of Fullerite C60 under Pressure

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Earlier [1, 2] we have reported on bulk synthesis of the hexagonal close packed (H.C.P.) phase of fullerite C60, which made it`possible to investigate the properties of this phase in more detail. Since the H.C.P. phase is less stable than the “standard” face-centered cubic (F.C.C.) phase, the synthesis of the H.C.P. phase required for special conditions (a set of solvents, temperature, etc). A series of problems should be solved to determine the range of stability of the H.C.P. phase, parameters of the transition of H.C.P. to F.C.C., and the mechanism of formation of the hexagonal packing the C60 molecules. In this work, the pressure-treated H.C.P.-C60 samples were studied and their properties were compared with those of the F.C.C.-C60 samples.

The volume properties of fullerite were studied up to 2.5 GPa at room temperature using a “piston-cylinder” high-pressure instalation. The dV/dP curves for H.C.P.-C60 and F.C.C.-C60 samples coincided within experemental errors that is a consequence of the identity of the corresponding elasticity constants and small values of additional constants for the H.C.P. phase. The intensities of the H.C.P. phase reflexes in the X-ray diffraction pattern weakened with pressure and virtually disappeared at 2.5 Gpa; i.e. the H.C.P. phase transformed into the F.C.C. phase. However, according to the elasticity theory, such a transformation should not occur either in single crystal or in powder.

Nevertheless, the strains causing the transformation H.C.P. structure into the F.C.C. can be brought about by compressing the H.C.P. single crystal in direction of one specific axis. Since the crystallites are chaotically arrangrd in powder, it is possible that the sample can be textured under the pessure, the crystals turning to be oriented in the wanted direction with respect to the power vector.

It should be noted that the H.C.P. – F.C.C. transition was not detected at heating in vacuum up 1100 K, when the cage of C60 molecule starts to destroy.

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References

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