Nanocomposites and nanomaterials

CO molecules physical and chemical sorption influence on structural properties of fullerite C_{60}

V.V. Meleshko, I.V. Legchenkova, Yu.E. Stetsenko, A.I. Prokhvatilov

B.Verkin Institute for Low Temperature Physics and Engineering, Natl. Acad. of Sci. of Ukraine, Prospect Nauky, 47, Kharkiv, 61103, Ukraine
E-mail: meleshko@ilt.kharkov.ua

Recently binary systems such as C_{60}-CO attract attention because of the possibility to create new substances and nanomaterials. Fullerite C_{60} has a cubic fcc structure which includes a sufficiently large octahedral (4,2 Å) and tetrahedral (2,2 Å) voids. It enables changing properties of fullerite in a wide range by varying a filling concentration of different interstitial impurities in the voids, for example, atoms of inert gas, simple molecular substances (H_2, N_2, O_2, CO, CH_4 etc.). At high temperatures and pressures in the systems fullerite – gas of simple molecules is possible synthesis of new substances. The cause of it is the change from the diffusion mechanism of physical sorption to a direct chemical interaction of impurity atoms with the atoms of carbon in the C_{60} molecules.

The influence of CO gas sorptions on structural characteristics of the mono- and polycrystalline fullerite C_{60} investigated by X-ray diffraction methods in temperature range 150-600 ^{o}C under pressure 30 atm. Sorption kinetics was studied by construction of C_{60} lattice parameter dependences from saturation with CO molecules time. Carbon monoxide dissociation at a temperature T > 300 ^{o}C was found. That dissociation is accompanied by carbon powder deposition and chemical interaction of atomic oxygen with C_{60}, CO and, probably, with condensate of carbon. These processes affect the structural characteristics of fullerite, which lead to non-monotonic saturation temperature dependence of the matrix lattice parameter and volume. In the area of physical sorption for two saturation regimes (150 and 250 °C) was determined concentration of solid solutions for $C_{60}(CO)_x$ poly- and single crystal samples. A linear effect of CO impurity molecules on the C_{60} lattice parameter and the temperature of orientational transition was established.