Vibration states of micro- and nanocarbon: structural aspects

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Carbon in a condensed state is polymorphic, which is determined by the possibility of the realization of different types of hybridization for valence electron orbitals: carbine (sp^1-), graphite (sp^2-), and diamond (sp^3-). In the indicated carbon systems, the physical properties vary from typically metallic to dielectric ones. Atoms in structural motives of GC and PC are in various hybridization states: sp^n- ($1 \le n \le 3$).

Phonon's structure of amorphous and crystal carbons is investigated in detail in Raman spectra. However, not all vibration states in view of an alternative selection rule are active in Raman spectra. Research of vibration states in IR-spectra of the condensed carbon is complicated by intensive not selective absorption of free carriers of a charge. The phonon spectrum in a series of nanocrystalline glassy carbon (GC) and microcrystalline pyrolytic carbon (PC) with the monotonously changing perfection degree of crystal structure is investigated in this work. Thermal processing of samples in the inert environment in the region of temperatures 1300–3000°C has allowed to change the sizes of fragments of coherent dispersion in a range 2, 5–800 nm. The natural surface of samples was investigated at a corner of reflection 20° on IFS-88 (Bruker) spectrometer in wide spectral area: 5000-400 cm^{-1} with the accuracy of 2 cm^{-1} and in a regime of accumulation up to hundred scans.

According to the theoretical-group analysis of fragments of crystal structure in IR- and Raman spectra of GC and PC should possess the optical activity intraplane and in plane vibrations of carbon atoms of graphite (D_{6h}^4) or fullerenes (I_h) mesh frame structures [1]. Selective absorption bands of vibration states E_{1u}, A_{2g}, T_{1u} in the aria of 1600-1300 cm^{-1} and A_{2u} - in the aria 900-800 cm^{-1} are registered in experimental IR-Fourier reflection spectra of GC and PC samples. Intensity and position of absorption bands considerably changed with the growth of temperature of samples processing and correlated with results of the structural researches, results of Raman and ATR (attenuated total reflection) spectra on the given objects [2].

[1] Carbon molecules and materials./Ed. by R. Setton, P. Bernier, S. Lefrant. - L.- N.Y.: Taylor and Francis. - 2002, 489 p.

[2] Bekhterev A. N. Vibration states in solid state carbon and nanocarbon. - Magnitogorsk: MaSU, 2007.