Optical characteristics of porous nanocarbon materials in effective media model: Bruggeman aprocsimation

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Practically all physical and many physical and chemical properties of condensed carbons be described on the basis of the information on a dispersion optical indexes in the region of electronic and phonon energy states of known forms crystal and amorphous carbons within the limits of the certain modeling representations. Method of the classical dispersive analysis, Kramers-Kronig method and effective media theory are used for calculation of a spectrum optical parameters *n(v)* and æ*(v)* (*ñ = n – i*æ)˜ of pyrolitic carbon (PC) and glassy carbon (GC) similar on structure with nanocrystalline graphite. Calculated infrared absorption spectra of PC and GC are compared to the similar data received from of in situ attenuated total reflection spectra (ATR) for samples in the region of vibration mode E_{1u} and A_{2u} of graphite. Process of reception of the sample has provided the minimal maintenance of impurity which averaged 0,001% of mass and high level of micro- and nanoporosity – till 50%.

We calculated n_{eff} using the theory, which describes effective dielectric properties of a granular composite with one kind of particles embedded randomly in a large volume of a host component. The effective media approximation also called Bruggeman's theory is the method to describe the effective dielectric properties of composites in which the particles of all components randomly mix together. This theory has been widely used to explain the dielectric and optical properties of composite materials and proved valid at all concentrations [1, 2]:

$$f\frac{\varepsilon_m-\varepsilon_k}{\varepsilon_m+2\varepsilon_k}=(1-f)\frac{\varepsilon_{eff}-\varepsilon_k}{\varepsilon_{eff}+2\varepsilon_k}$$

where ε_{eff}, ε_m, ε_k – effective, matrix, embedded component indexes of samples, f – volume fraction of embedded component. The obtained spectra of GC and PC well describe the experimental infrared reflectance data of the samples in spectral region 2000–1000 cm^{-1} [3].

[1] Carbon Molecules and Materials, Ed. by R. Setton, P. Bernier, and S. Lefrant.- Taylor & Francis, New York, 2002.
[2] Bekhterev A. N. Vibration states in solid state carbon and nanocarbon. - Magnitogorsk: MaSU, 2007.
[3] Bekhterev A.N., Zolotarev V.M., Yakovlev V.B., *Opt. Spektrosk.* **59**(5), 1057 (1985).