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Comparative analysis of the refractive and spectral properties of the potassium bromide with boron-nitride nanotubes interface

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The analysis of the refractive and spectral properties of the potassium bromide with the boron-nitride nanotubes interface is carried out. The most optimal type of the chirality of the boron-nitride nanotubes in the entire spectral range studied was revealed, which is established from the calculations performed for the dispersion dependences of the refractive index of the boron-nitride nanotubes with different chirality, as well as from the evaluation of the dispersion dependences of the reflection coefficient at the KBr-BNNT interface with different chirality.

Keywords: spectral range, refractive index, interface, reflection spectra.

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Introduction

In recent years boron nitride nanotubes (BNNT) have attracted the attention of researchers due to their significant semiconductor gap [1] and high structural stability which makes this material suitable for use in photoluminescent devices [2]. The electronic and structural properties of BNNT have been theoretically studied in detail. Dependence of the width of the BNNT forbidden region was studied as the function of internal diameter and nanotube chirality. A strong decrease in the gap was observed for nanotube diameters less than about 1.3 nm. The calculations of minimal lattice energy conducted by Hernandez et al. show that the most favorable chirality for BNNT is zigzag [4]. They also predicted the Young's modulus of about 300 GPa for zigzag-shaped and armchair nanotubes and a certain degree of bending perpendicular to the nanotube axis. There are a lot of experimental

works performed using transmission electron microscopy (TEM) [5–14], and much fewer articles on the electronic and optical properties of BNNT samples. This is, for example, the IR response of BN vibrations in BNNT which can be used to characterize nanotube samples. BNNT were first obtained by methods of arc discharge and laser ablation. Most produced BNNT have a zigzag-shaped geometry.

Nowadays there is great interest in boron nitride nanotubes due to their electronic [15–17], thermal [18–21] and mechanical properties [22, 23] which in many cases differ or are superior to similar parameters of carbon nanotubes. The analysis of IR spectroscopy with Fourier Transformation is conducted using infrared spectrum analyzer in the wave numbers range of 4000–500 cm⁻¹, relative to the KBr crystal matrix. As shown in fig. 1a,b, with similar absorption curves in BNNT we can observe characteristic peaks at 1380 cm⁻¹ and 800 cm⁻¹

due to fluctuations in the B-N bond, parallel and perpendicular axis, respectively [24]. Both peaks demonstrated a strong IR-response which is observed in IR reflecting power.

Spectrum presented in fig. 1c shows strong fluctuations at 1375 and 793 cm^{-1} , which are characteristic for primary and secondary absorption curves of BNNT, respectively. Absorption band at 1375 cm^{-1} is related to the well-known planar vibrational mode (E_{2g}) BNNT, while weak absorption bands at 793 cm^{-1} correspond to the out of plane vibration [25]. Both the spectrum profile and absorption curves

are similar to those reported for BNNT which additionally confirms that unprocessed products are BNNT.

Absorption spectra of BNNT (fig. 1d), show sharp absorption peak at 204 nm . Light absorption property and width of the BNNT forbidden zone were investigated using spectroscopy operating in the reflection mode, as shown in fig. 1e. Reflection spectra in the UV-visible range show two absorption bands at 266.4 nm (4.65 eV) and 214.2 nm (5.79 eV) corresponding to the exciton absorption and optical absorption at the BNNT band edge [25].

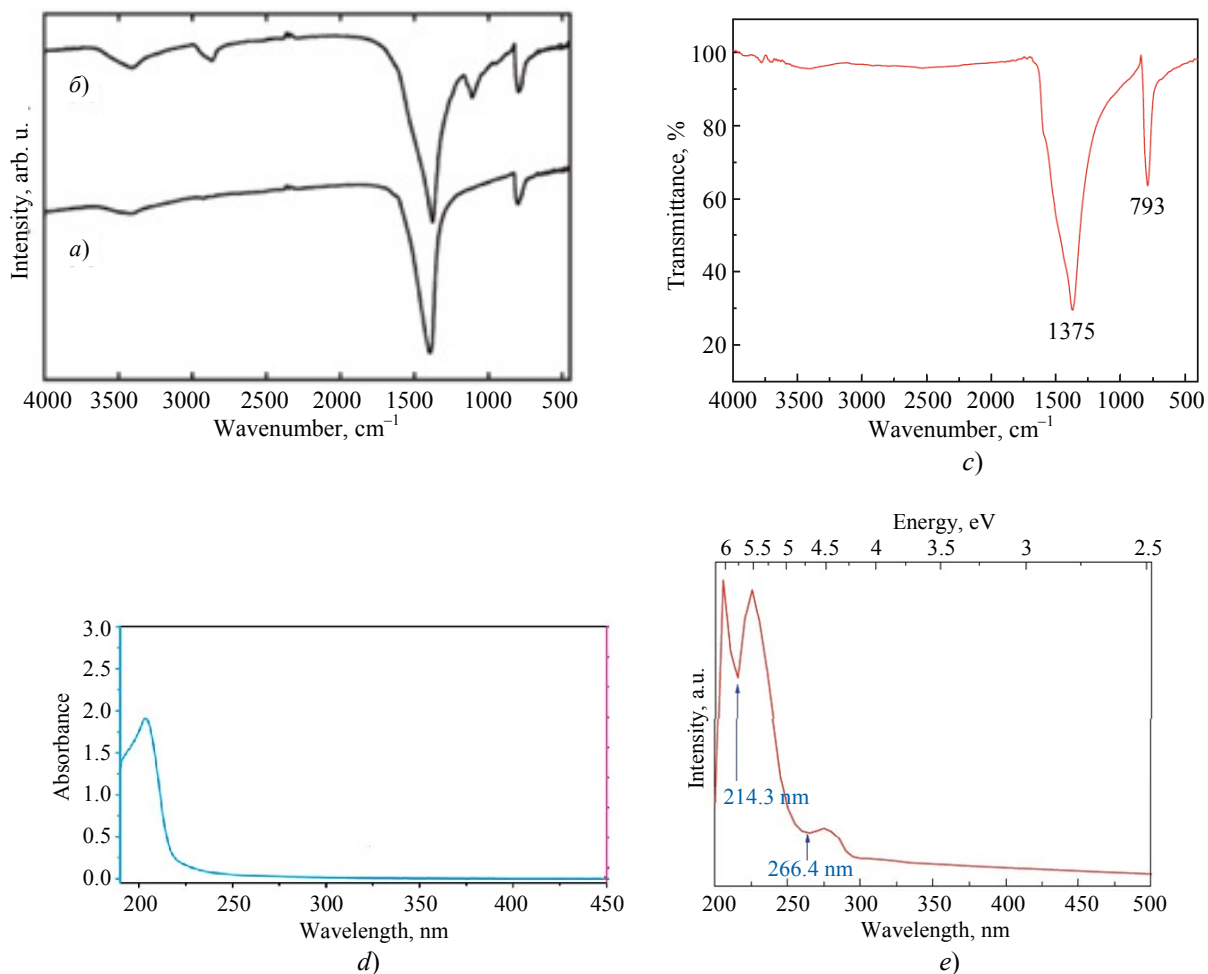


Fig. 1. Infrared Fourier transmission spectrum of the original (a) and restored (b) boron-nitride samples in the KBr [26] matrix, (c) transmission spectrum BNNT (d) absorption spectra in the BBNT UV-visible range (e) reflection spectra in the BBNT UV-visible range [25]

Refraction index models

Dispersion characteristic of the KBr refraction index is well-known and approximates as follows [27]:

$$n^2 = 1.39408 + \frac{0.79221\lambda^2}{\lambda^2 - (0.146)^2} + \frac{0.01981\lambda^2}{\lambda^2 - (0.173)^2} + \frac{0.15587\lambda^2}{\lambda^2 - (0.187)^2} + \frac{0.17673\lambda^2}{\lambda^2 - (60.61)^2} + \frac{2.06217}{\lambda^2 - (87.72)^2} \quad (1)$$

Here λ is wavelength expressed in μm .

By using the calculation method presented in studies [27–29], the following calculations were performed in this study.

It is shown (fig. 2) that the refractive index of nanotubes based on boron nitride depends on the chirality (armchair, zigzag-shaped, chiral).

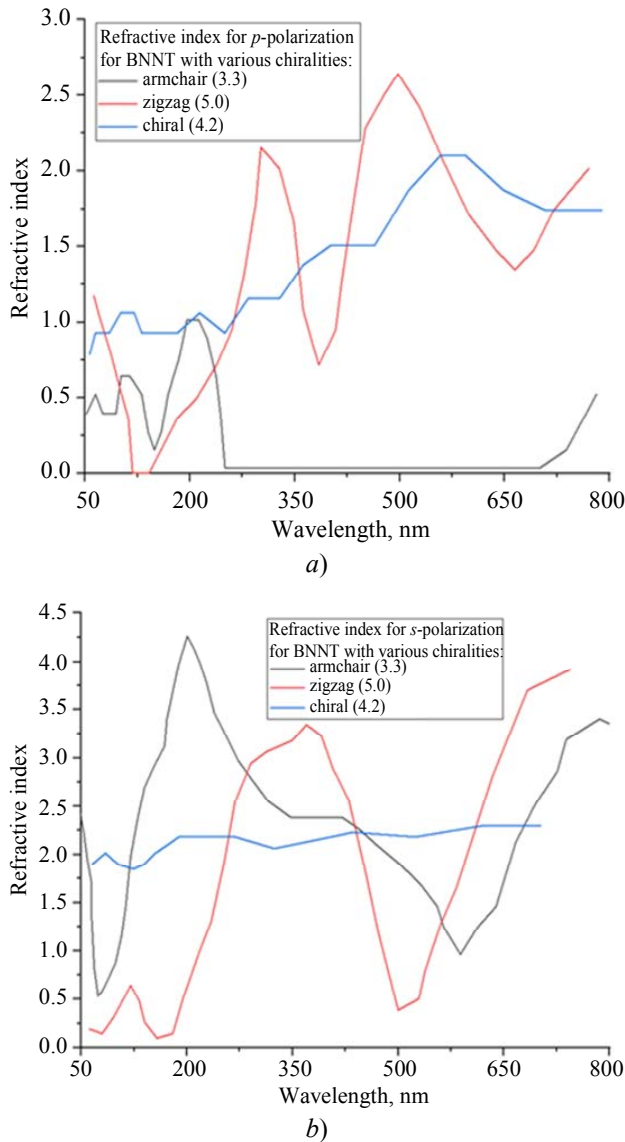


Fig. 2. Dispersion dependencies of the BBNT refractive index with different chirality for p-polarized (a) and s-polarized (b) radiation in the spectrum range of 50–800 nm

The obtained refractive properties of BBNT with different chirality types do not contradicts the data of publications [30–34] where optical properties of such structures have also been studied.

Reflection spectrum models

Continuing to study the spectral parameters of BNNT, we have also calculated reflection losses at the interfacial area of KBr-BNNT (fig. 3) using the Fresnel's formula (2) for normal incidence:

$$R(\lambda) = \left(\frac{n_{\text{KBr}}(\lambda) - n_{\text{BNNT}}(\lambda)}{n_{\text{KBr}}(\lambda) + n_{\text{BNNT}}(\lambda)} \right)^2 \quad (2)$$

Here n_{KBr} and n_{BNNT} are refraction indices for KBr (see expression 1) and BNNT (from the data from fig. 2) that depend on the wavelength λ .

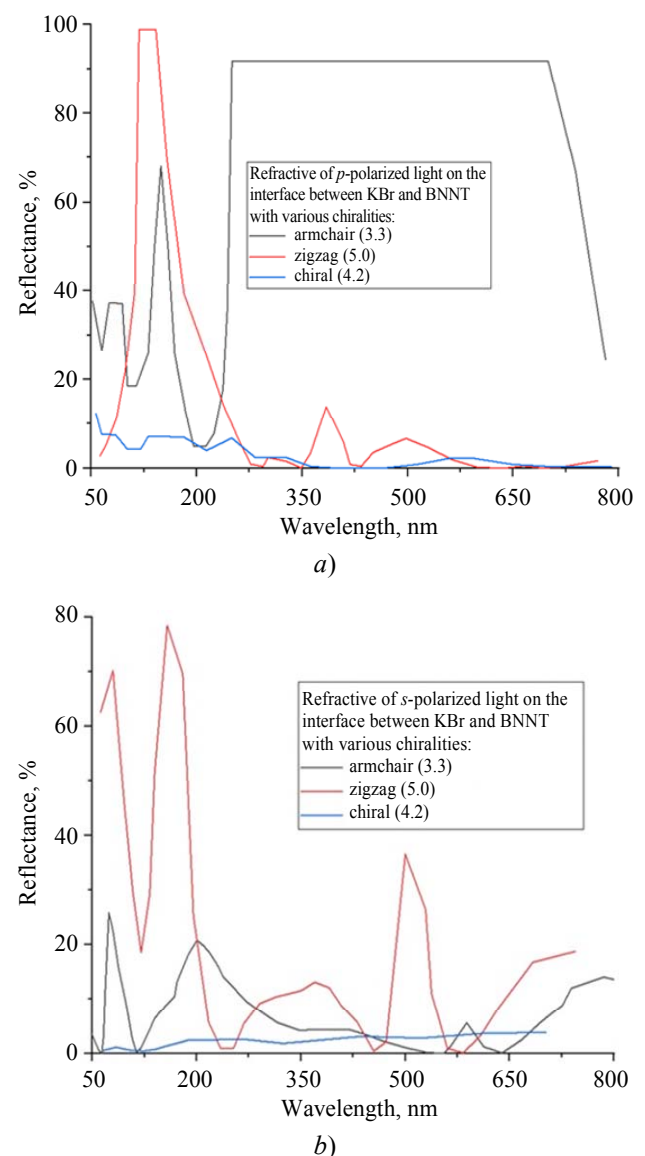


Fig. 3. Dispersion dependencies of the reflection coefficient at the interfacial area of KBr-BNNT with different chirality for p-polarized (a) and s-polarized (b) radiation in the spectrum range of 50–800 nm

It should be noted that when selecting the chirality of nanotubes, BNNTs with chirality (4,2) were selected, similarly to [35]. Based on the analysis of publications [36–40] of different BNNT types, this type of nanotubes has a more optimal atomic configuration.

Conclusion

From the calculations performed for the dispersion dependencies of the BBNT refractive indices with different chirality, as well as from the assessment of dispersion dependencies of the reflective coefficient at the KBr-BNNT interfacial area with different chirality, it was established that the most stable properties in the entire studied spectral range (from X-ray to the near infrared) are boron–nitride nanotubes with chirality (4,2).

It was shown that for further calculation of energies of chemical bonds and optimization of structures it is more preferable to use boron–nitride nanotubes with chirality (4,2) the reflection spectra of which differ by no more than 10 % from the calculated and predictable ones in both polarizations and spectral range from 50 to 800 nm.

The studied nanostructured material can be used as new structural material for spectroscopy, for example, when optimizing the polarization of potassium bromide plane-parallel plates in X-ray apparatus. Low reflection may be a priority here for the selected spectral range. The conducted study will be useful in the training process when studying the properties of nanostructural composites functioning not only in the visible spectrum but also in the area of IR-spectrum.

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