Optical properties of alkali halide crystals

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Abstract. The results of measuring the transparency bands in a wide wavelength range - from UV to 3000 μm for crystals of sodium chloride (NaCl), potassium chloride (KCl), iodine bromide (KBr) and rubidium iodide (RbI) are presented. It was shown that, along with well-known data on the transparency of these crystals in the UV and IR ranges, they have a transmission zone in the THz range in the region of 1000 μm.

1. Introduction
Alkaline halide crystals are widely used in the optics of IR range. However, they are also interesting for use in other ranges. With the discovery of lasers, optical instrumentation began to develop rapidly, and it became possible to study the spectral characteristics of materials in the far IR and THz ranges. Recently, there has been significant interest in these ranges, since they are of great interest for a number of fundamental (chemistry, physics, astronomy) and applied fields. Many materials, including textiles, plastics, and biological textile, are transparent in these ranges. Terahertz radiation due to the low photon energy can be widely used in medical diagnosis, as well as for quality control and / or for security assurance without damaging the material [1]. Until recently, technologies for generation, conversion, and registration of this region of the spectrum lagged noticeably from neighboring ranges. However, this lag is reduced in recent years. A variety of radiation sources, including laser ones, at which significant power levels have already been obtained (up to 109 W per pulse), have been created [2, 3]. Nevertheless, the development of this range is noticeably inhibited due to a significant deficit of high-quality transparent optical materials [4-6]. In the present work, we report on an experimental study of the optical properties of some alkali halide crystals in a wide range of wavelengths - from UV to 3000 μm. This work is a continuation of our studies [4-6].

2. Materials and methods of the experiment technique
Since alkali halide crystals are actively used in IR optics, in this work samples of industrial materials were used. Climatic and mechanical properties of single crystals considered in this work are very low. Alkaline halide crystals are very fragile crystals that easily crack by cleavage (along the <100> planes). They are water-soluble, and work with them is possible only in conditions of low humidity or after applying moisture-proof coatings. The spectral transmission of fabricated research samples with a thickness of 2 mm was recorded using a Photon RT spectrophotometer from Essent Optics, Bruker Vertex 70 Fourier spectrometers and
Bruker IFS 66v/s in the spectral range of 0.9 - 670 μm, and in the range of 150 - 3000 μm - with a TeraK8 MenloSystems device. It should be noted that the last device in the range of 100 - 1500 microns provides the ability to conduct quantitative measurements; in the range of 1500 - 3000 microns, only high-quality measurements are provided.

3. Experimental results and discussion

The results of optical transmission measurements for crystals of sodium chloride (NaCl), potassium chloride (KCl), iodine bromide (KBr), and rubidium iodide (RbI) are presented in this work. For a sodium chloride crystal, it was found, that after a transparency band in IR region, a wide absorption band of 15 – 500 μm is observed. Further, up to the region of 3000 μm, the crystal is completely transparent. Similar results were obtained for other crystals. For KCl, the phonon absorption band was 25 - 1000 μm, for KBr - 35 - 600 μm, for RbI - 55 - 1000 μm. The decrease in transmittance in the THz region, compared with the IR region, is explained by both an increase in Fresnel reflection due to an increased refractive index and some increase in the absorption coefficient.

Figures 1–4 show the results of experimental study of the transmission, reflection, and calculated values of the attenuation and refraction coefficients of these crystals. Figure 1 shows the spectral dependence of the transmission and attenuation coefficient for KBr.

In the region of phonon absorption, the region of anomalous change in the reflection coefficient of crystals is of interest. Figure 2 shows the spectral dependence of transmission and reflection of NaCl single crystals. In the region of the beginning of the phonon absorption band, the reflection coefficient, as follows from the Madelung model, is close to zero, and further (in the range of 50 - 60 μm), a reflection peak is observed - almost 90%. These effects also occur in other alkaline halide crystals, however, the absolute values of the corresponding wavelengths differ, which makes it possible to vary the practical application of these properties.
Figure 3 shows the transmission spectrum and dispersion of the refractive index of sodium chloride (NaCl) single crystal, and Figure 4 shows the spectral dependence of the transmission of rubidium iodide (RbI) single crystals. Figures 1 - 4 clearly shows that after the transmission band in the IR region, in all of the described crystals, the region of intense absorption due to phonon processes [7] is observed. At the same time, it is noticeable, that the edge of the onset of phonon absorption, as a rule, shifts to the region of longer wavelengths. Further, in the THz region, near a wavelength of ~ 1 mm, the absorption noticeably weakens and an increase in transmission is observed.

![Figure 2](image.png)

**Figure 2.** Spectral dependence of the transmission (a) and reflection (b) of KCl single crystals

The maximum long-wavelength transmission in the IR range is observed for RbI crystals (Figure 4). It should be noted that thin plates of RbI crystals are transparent from 0.24 μm to 64 μm [8], but they are still rarely used in optics due to the higher hygroscopicity and cost than KBr and CsI. However, one should pay attention to these crystals due to the development of optics in this range. So far, RbI crystals are used in high-energy particle detectors [9]. Figure 4 shows the RbI spectrum, the intense absorption band of which in the region of 7 - 8 μm is caused by an impurity of barium (Ba), introduced specifically to improve the scintillation properties of the crystal. This impurity practically does not affect the transmission of the crystal in other areas.

4. Conclusions

In this work, the spectral dependences of the transmittance of NaCl, KCl, KBr and RbI in the range from 0.2 to 3000 μm were experimentally obtained. It was found that in the millimeter region in these crystals a transparency zone is observed, which makes it possible to use these materials in devices of the THz range.
Figure 3. Spectral dependence of the transmission (a) and reflection coefficient (b) of NaCl single crystals

Figure 4. The transmission spectrum of RbI single crystals. This sample had a thickness of 6.78 mm

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