

# Thermal diffusivity of BaLiF<sub>3</sub> crystals

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## Abstract

BaLiF<sub>3</sub> crystals doped with transition metal ions are potential new laser active media. Thermal diffusivity of a pure BaLiF<sub>3</sub> crystal was determined at room temperature using the photoacoustic two-beam phase lag method, which consists in measuring the relative phase-lag for the photoacoustic signal between rear and front surface illumination at a single modulation frequency.

## 1. Introduction

The thermal diffusivity  $\alpha$  is the parameter that provides the rate at which heat flows through a medium. Knowledge of this parameter is very important in crystal growth, laser engineering and photoacoustic spectroscopy studies. Thermal diffusivity is related to thermal conductivity  $K$  through the equation  $\alpha = K/(\rho C)$ , where  $\rho$  is the density and  $C$  is the thermal capacity at constant pressure. In this way it is possible to determine the thermal conductivity from the thermal diffusivity once  $\rho$  and  $C$  are known.

In this paper we report on the determination of the thermal diffusivity value for pure BaLiF<sub>3</sub> crystals at room temperature. BaLiF<sub>3</sub> crystals are important materials since, when doped with transition metal ions, they are a potential new laser host. BaLiF<sub>3</sub> crystals are an "inverse" perovskite with cubic structure (space group O<sub>h</sub><sup>1</sup>-Pm3m), where the monovalent ion Li<sup>+</sup> is at the center of six F<sup>-</sup> octahedrons, whereas the Ba<sup>2+</sup> divalent ions are in the 12-fold environment site, resulting in a different crystal field interaction from the classic perovskite structure [1]. The recent interest in this material is due to its expected tunable laser action in the infrared region at room temperature.

## 2. Methodology

The applied methodology (photoacoustic two beam phase-lag method [2, 3]) involves measuring the relative phase-lag between rear and front crystal surface

illumination at a single modulation frequency using conventional photoacoustic spectroscopy. Photoacoustic signal generation is described using the Rosencwaig and Gersho (RG) thermal diffusion model [4, 5], giving the phase-lag  $\Delta\phi$  as a function of the sample thickness  $l$  and the thermal diffusion length  $\mu$ :

$$\tan \Delta\phi = \tan(l/\mu) \tanh(l/\mu) \quad (1)$$

with  $\mu = \sqrt{(2\alpha/\omega)}$  where  $\omega$  is the illumination modulation frequency.

The restrictions of the applied model are to consider that all the incident light is absorbed at the surface, and to assume that the heat flux into the surrounding air is negligible. For this reason optically opaque absorbing layers have to be provided, by thin film deposition for example.

## 3. Experimental details and results

The pure BaLiF<sub>3</sub> crystal [6] was grown by the Czochralski method. The sample studied was 1.0 × 1.0 × 0.03 cm<sup>3</sup>. The sample thickness was chosen in order to ensure that the thermal oscillations due to rear and front illumination are of the same order.

A Kr laser with 0.5 W power, modulated at 40 Hz, was used as the excitation light. The photoacoustic cell employed was of the gas-microphone type (Fig. 1), with a commercial electret microphone, whose output was measured using a lock-in amplifier. The sample had both faces coated with silver paint, with a layer thickness of the order of 60 μm, to ensure that all the incident light would be absorbed at the crystal surface. As the thermal diffusivity for silver paint is considerably

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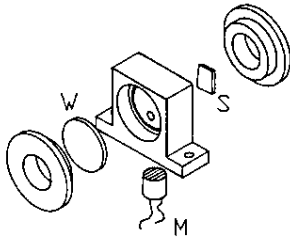


Fig. 1. Schematic drawing of the photoacoustic cell: S sample; W window; M microphone.

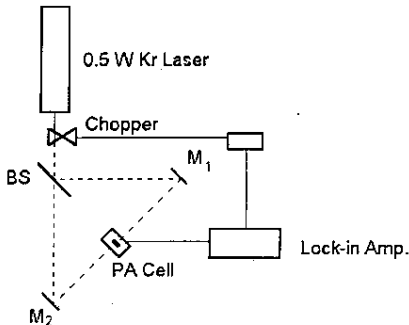


Fig. 2. Experimental set-up: BS beam splitter; M<sub>1</sub> and M<sub>2</sub> mirrors.

higher than for ionic crystals, the phase-lag for these layers can be neglected.

The experimental apparatus shown in Fig. 2 was evaluated by measuring the thermal diffusivity of a pure LiF crystal. The value obtained was  $0.032 \pm 0.005 \text{ cm}^2 \text{ s}^{-1}$ , whilst the tabulated value is  $0.038 \text{ cm}^2 \text{ s}^{-1}$  [7].

For the BaLiF<sub>3</sub> sample the thermal diffusivity value determined was  $\alpha = 0.037 \pm 0.005 \text{ cm}^2 \text{ s}^{-1}$ .

There are no values available in the literature for comparison, but this value was expected to be close to that for LiF crystals, the starting material in the growth process of BaLiF<sub>3</sub> crystals.

This result can be used for the doped BaLiF<sub>3</sub> crystals considering that, for ionic crystals at room temperature, the main mechanism responsible for heat transport is umklapp scattering (phonon-phonon), which is independent of the impurities or defects present in the crystal [8].

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