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TEMPERATURE ASPECTS OF A CUBOID CRYSTAL IN PHOTOACOUSTIC INTERACTION

When a solid crystal undergoes photoacoustic effect, excitation process occurs due to a fraction of incident radiation absorbed by that sample. The nature of excitation depends on the energy of incident radiation. The relaxation processes, generally non-radiative in nature, are observed. Alternate processes of absorption and non- radiative relaxation cause variation in translational temperature in atoms of the crystal. In this paper, the thermal aspects of an isotropic cuboid crystal of elastic material in photoacoustic interaction are presented. This theoretical determination is carried out by applying the finite Marchi–Fasulo integral transform method within the crystal size limitations of a homogeneous cuboid crystal. The results are obtained in terms of infinite series, and the numerical calculations are carried out by using MATHCAD-7 software. The transient translational temperature on the surface of the cuboid crystal in photoacoustic interaction is mathematically determined in terms of thermal conductivity of the elastic material of the crystal.

Keywords: *cuboid crystal, photoacoustic cell, photoacoustic effect, Marchi – Fasulo integral transform, transient translational temperature.*

1. Introduction

Today, crystalline solids are widely used in industries because of their wide applications. Their great practical importance has attracted researchers for finding new scopes. Elastic parameters of crystals are studied to discover their applicability. Crystals of better quality and large size are prepared artificially for their practical use. Thermal aspects of crystals are of great importance since they are related to their strength and fragile nature.

In photoacoustic interaction with a crystal, electromagnetic radiation is absorbed by molecules of the sample crystal. Electromagnetic radiation leads to the crystal warming-up in that area. During the relaxation processes by non-radiative way, the molecular collisions occur. Thermal expansion of the crystal creates pressure fluctuations, which can be detected as ultrasonic waves or an acoustic signal [1]. In other words, the conversion of an optical signal into an acoustic signal takes place in a photoacoustic effect [2]. The solid crystal absorbs a fraction of the radiation falling upon it, and an excitation process occurs. The excitation type depends on the energy of the incident radiation.

Relaxation processes, which are also known as non-radiative de-excitation processes, are typical for the considered processes. The light–matter interaction is responsible for heat generation within a solid crystal. In the experiments, when modulated incident radiation is used, it has been observed that the thermal energy generation within the crystal becomes periodic. A pressure wave or a thermal wave is produced [3] that has the same frequency as the modulation of the incident radiation. The pressure wave or the thermal wave transfers energy towards the sample boundary. As a result, the periodic temperature change is observed. The temperature varies on the crystal surface, and the variations are periodic in nature. This process results in the acoustic signal generation in the gas around the solid sample. This sound wave travels through the surrounding volume of the gas to a detector. The detector may be a piezoelectric transducer, a microphone, or an optical method at the place where the signal is produced. The signal from the detector or microphone is plotted as a function of the wavelength, and it gives the spectrum that is proportional to the absorption spectrum of the sample [4–6]. This principle of photoacoustic effect can be schematically represented as shown in figure 1.

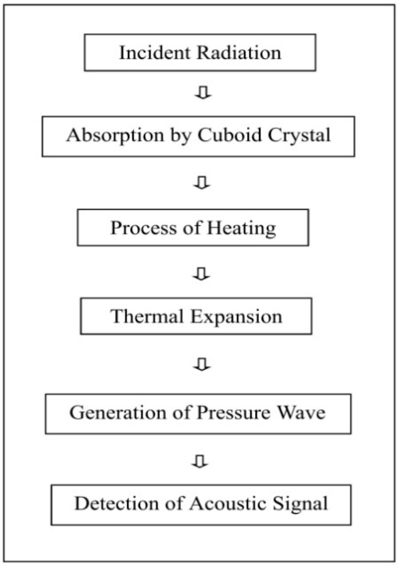

Fig. 1. Processes in Photoacouslic generation in a cuboid crystal

However, very little attention has been paid by researchers to the thermal stress determination during photoacoustic analysis. The main purpose of the present work is to determine mathematical aspects of the transient temperature generated in a cuboid crystal in photoacoustic effect.

Initial theoretical explanation of temperature of solids during photoacoustic interaction was presented by Rosencwaig in 1975 [7]. He correlated the temperature of the sample with thermal conductivity, density and specific heat of the sample undergoing photoacoustic investigation. Later, in 1976, a one-dimensional model of the heat flow and temperature was formulated by Rosencwaig and Gersho [8]. They derived mathematically the temperature distribution in a cell with a solid sample. McDonald and Wetsel published temperature calculations of photoacoustic interaction in a three-dimensional model with restrictions on thermal waves in the transverse direction [9]. They presented a composite piston model and proved its validity for thermally thick samples. Quimby and Yen primarily calculated the surface heat transfer in temperature estimation [10]. Chow developed a three-dimensional model in a general way without any restrictions on the sample size in a photoacoustic cell [11]. He showed that for an incident beam with a narrow focus, the analysis of the Gaussian beam profile indicated an insignificant role of the spot size. In the recent years, Merzadinova et al. calculated ambient temperature of a solid in thermal diffusivity determination of structurally inhomogeneous, multilayer, and composite solids in photoacoustic interaction [12]. The work was based on the fundamental Rosencwaig–Gersho model by using laser flash method. Though a large number of research papers have been published regarding photoacoustic interaction till date, the theoretical presentation of temperature aspects of a homogeneous and isotropic crystal, which is cuboid in shape, have not been presented yet. This paper presents such theoretical estimation.

2. Photoacoustic effect

In photoacoustic effect, interaction of electromagnetic radiation with matter generates sound. This effect represents the absorption of incident radiation by a target molecule. Photoacoustic effect is popular due to a minimal sample preparation during execution and an ability to examine scattering and opaque sample along with the capability to access a depth profile [13]. These features enable photoacoustic spectroscopy to be used for monitoring of various gases as well as for depth-resolved characterization of solid crystals [14]. The energy absorbed by the solid crystal can be measured by pressure fluctuations generating shock pulses or sound waves [15]. In photoacoustic spectrum, a plot of the intensity of the detected acoustic signal against the excitation wavelength is analyzed. The sound waves are detected by a piezoelectric detector or a microphone.

In 1880–1881, Alexander Graham Bell [16] discovered the way the light interacts with solid. He observed that, when the mechanically chopped sunlight falls on a thin disk, sound waves were generated. The similar effect was observed, when infrared or ultraviolet light was used. It is called the photoacoustic effect. A plot of the sound loudness against the wavelength of the light used is called a photoacoustic spectrum. According to Haisch and Niessner [17], this effect captured the interest of scientists worldwide when researchers led by Allen Rosencwaig at Bell Labratories rediscovered the phenomenon.

3. Photoacoustic interaction in a cell

The photoacoustic interaction is generally carried out in a small structure having an air-tight arrangement with a sensitive acoustic sensor. Such a cell is termed as a photoacoustic cell [18]. The sensor is embedded into one of the walls of the cell. When the periodic variations in temperature occur at a respective point of the surface of the solid crystal [19–20], an acoustic wave is generated in the gas [21]. This wave travels through the volume of the surrounding gas to a detector. This detector converts it into equivalent electrical signals. The detector may be a piezoelectric transducer or a capacitance transducer [22] in the adjoining gas phase of the crystal. This clearly shows that the photoacoustic signal is a result of two types of the processes taking place in the crystal. These processes are the absorption of electromagnetic radiation, expressed by the absorption coefficient B, and the propagation of thermal energy in the solid crystal which is specified by the thermal diffusivity, α.

The crystal under execution has an important parameter, known as the optical absorption length [23]. It represents the depth up to which total incident radiation is absorbed in the crystal. Due to this absorption, the resulting thermal wave generated in the crystal becomes heavily damped. This wave can be considered as a fully damped in a specific distance of $2\pi\mu_s$. Here, μ_s is the thermal diffusion length. It is generally assumed that the thermal waves, which originate from a depth less than or equal to μ_s, make significant contribution to the photoacoustic signal generated. The thermal diffusion length is dependent on the thermal diffusivity as well as the modulation frequency ω of the incident radiation. All these parameters can be expressed by the following relation:

$$\mu_s = \sqrt{\frac{2\alpha}{\omega}}. \quad (1)$$

This formula is very important, because if the modulation frequency ω is changed, then for a given solid crystal with known thermal diffusivity, the examined depth μ_s may also be changed.

The resulted photoacoustic signal is of complex nature because it has a magnitude and a phase related with the modulation of the incident radiation. Since the thermal characteristics of the solid crystal and the modulation frequency are dependent on the absorption coefficient, the resulting photoacoustic signal is directly proportional to the power of the incident radiation. This signal also depends on the characteristics of the gas surrounding the solid crystal surface. The properties of the material that backs the crystal also play an important role for the photoacoustic signal.

4. Arrangement of a cuboid crystal

Consider a cuboid crystal made of thermoelastic material is inserted into a modified photoacoustic cell. The crystal is homogeneous and isotropic. This crystal is placed in a cylindrical cavity of the photoacoustic cell to produce a photoacoustic signal. The cell is air-tight, and, hence, it has a constant volume of the gas surrounding the crystal. The crystal is irradiated by a proper laser source. The crystal absorbs heat and generates the photoacoustic signal.

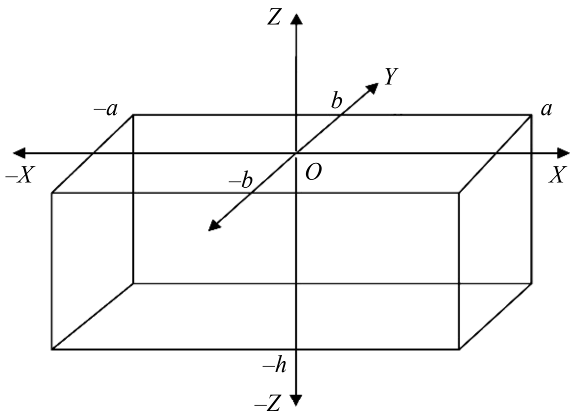

Fig. 1. Cuboid crystal in Photoacouslic interaction

Assume that the cubic crystal placed in the cell is occupying the space, as shown in figure 2. This space is mathematically defined as

$$\text{D}: -a \le x \le a\ ,\ -b \le y \le b\ .\ 0 \le z \le -h\ . \quad (2)$$

Consider a Cartesian coordinate system, in which the displacement components are u_x, u_y, u_z in *x*, *y*, *z* directions, respectively [24–25]. These displacement components can be expressed in the integral form as

$$u_x = \int \left[\frac{1}{Y} \left(\frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} - \nu \frac{\partial^2 U}{\partial x^2} \right) + \lambda T \right] dx , \tag{3}$$

$$u_y = \int \left[\frac{1}{Y} \left(\frac{\partial^2 U}{\partial z^2} + \frac{\partial^2 U}{\partial x^2} - \nu \frac{\partial^2 U}{\partial y^2} \right) + \lambda T \right] dy , \tag{4}$$

$$u_z = \int \left[\frac{1}{Y} \left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} - \nu \frac{\partial^2 U}{\partial z^2} \right) + \lambda T \right] dz , \tag{5}$$

where *Y*, ν, and λ are the Young modulus, the poisson ratio, and the coefficient of linear thermal expansion of the material of the crystal, respectively.

5. Temperature aspects

Consider that *U*(*x*, *y* ,*z* ,*t*) is the airy stress function [26] which satisfies the differential equation

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)^2 U(x, y, z, t) = -\lambda Y \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)^2 T(x, y, z, t) . \tag{6}$$

Here, $T(x, y, z, t)$ denotes the translational temperature of the crystal satisfying the following differential equation:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} + \frac{\theta(x, y, z, t)}{k} = \frac{1}{\alpha} \frac{\partial T}{\partial t}, \tag{7}$$

where k is the thermal conductivity and α is the thermal diffusivity of the material of the crystal. Let $\theta(x, y, z, t)$ be the heat generated within the crystal for $t > 0$ under initial conditions

$$T(x, y, z, 0) = F(x, y, z). \tag{8}$$

The finite Marchi–Fasulo integral transform of *f*(*z*) within the limitations $-h < z < h$ is defined as [27]

$$\overline{F} = \int_{-h}^{h} f(z) P_n(z) dz. \tag{9}$$

The Marchi–Fasulo transform technique is used to determine the unknown temperature, temperature distribution, displacement of the fields and thermal stresses on a plane surface of a thin object. Here, the determination of three-dimensional transient thermal parameters for a thin crystal made of elastic material is considered within the context of the theory of generalized elasticity. At each point within (-*h*, *h*), the function *f*(*z*) is continuous. Again, the inverse finite Marchi–Fasulo transform for previous conditions is defined as [28]

$$f(z) = \sum_{n=1}^{\infty} \frac{\overline{F}(n)}{\lambda_n} P_n(z). \tag{10}$$

Here,

$$P_n(z) = Q_n \cos(a_n z) - W_n \sin(a_n z),$$

$$Q_n = a_n(\alpha_1 + \alpha_2)\cos(a_n h) + (\beta_1 - \beta_2)\sin(a_n h),$$

$$W_n = (\beta_1 + \beta_2)\cos(a_n h) + (\alpha_1 - \alpha_2)a_n \sin(a_n h),$$

$$\lambda_n = \int_{-h}^{h} P_n^2(z)\,dz,,$$

$$\lambda_n = h\left[Q_n^2 + W_n^2\right] + \frac{\sin(2a_n h)}{2a_n}\left[Q_n^2 - W_n^2\right].$$

Eigenvalues a_n are the solutions of the equation

$$[\alpha_1 a\cos(ah) + \beta_1 \sin(ah)] \times [\beta_2 \cos(ah) + \alpha_2 a\sin(ah)] =$$

$$= [\alpha_2 a\cos(ah) - \beta_2 \sin(ah)] \times [\beta_1 \cos(ah) - \alpha_1 a\sin(ah)]. \qquad (11)$$

Here, $\alpha_1, \alpha_2, \beta_1, \beta_2$ are constants.

By applying the finite Marchi–Fasulo transform to boundary conditions and their inverses three times, we obtain

$$\frac{d\overline{\overline{T}}^*}{dt} + \propto q^2 \overline{\overline{T}}^* = \propto \left(\varnothing + \frac{\overline{\overline{\theta}}^*}{k} \right), \qquad (12)$$

where

$$\varnothing = P_m(a)F_2 - P_m(-a)F_1 + P_n(b)F_4 - P_n(-b)F_3 + P_l(h)f_2 - P_l(-h)f_1$$

and $q^2 = a_m^2 + a_n^2 + a_l^2$ is the eigenvalue. (13)

First order differential equation (12) has the following solution:

$$\overline{\overline{T}}^*(m,n,l,t) = e^{-\propto q^2 t}\left[\int_0^t \propto \left(\varnothing + \frac{\overline{\overline{\theta}}^*}{k} \right) e^{\propto q^2 t' dt'} + c \;\; , \; c = \overline{\overline{F}}^*(m,n,l) \right], \qquad (14)$$

$$\overline{\overline{T}}^*(m,n,l,t) = \int_0^t \propto \left(\varnothing + \frac{\overline{\overline{\theta}}^*}{k} \right) e^{\propto (a_m^2 + a_n^2 + a_l^2)(t-t')dt'} + e^{-\propto (a_m^2 + a_n^2 + a_l^2)t}\,\overline{\overline{F}}^*(m,n,l). \qquad (15)$$

If we apply the inverse finite Marchi–Fasulo transform to this equation with boundary conditions three times, we obtain

$$T(x,y,z,t) = \frac{k}{c^2}\sum_{m,n=1}^{\infty}\left[\frac{P_m(x)}{\lambda_m}\right]\left[\frac{P_n(y)}{\mu_n}\right]\left[\phi_1(z)\Psi_1(t) - \phi_2(z)\Psi_2(t)\right] +$$

$$+ \frac{2k\pi}{h^2}\sum_{l,m,n=1}^{\infty}\left[\frac{P_m(x)}{\lambda_m}\right]\left[\frac{P_n(y)}{\mu_n}\right]\left[\frac{l}{\cos l\pi}\right]\left[\frac{1}{1 + cl\pi^2}\right]\left[n_1(z)\Psi_3(t) - n_2(z)\Psi_4(t)\right]. \qquad (16)$$

6. Conclusions

Exact expression (16) for transient translational temperature on the surface of a cuboid crystal in photoacoustic interaction is mathematically determined using the Marchi–Fasulo method in terms of thermal conductivity of thermoelastic material of the crystal. This expression allows calculating of various parameters of the cuboid crystal such as the constants related with elasticity. Since various crystals are used in industrial applications at different temperatures, their ability to withstand a given temperature value for particular application is helpful when designing various scientific and industrial processes involving laser interactions. This mathematical approach constitutes an important step towards determination of various aspects of premature failure of solid state industrial components and devices. The proposed approach provides a theoretical basis for the study on the influence of stresses in photoacoustic interaction in various cuboid crystals. The obtained results are of great importance when studying optical and thermal properties of complex materials. This work can be used in future research for scientific and industrial applications.

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REFERENCES

1. McDonald F.A. (1980) Photoacoustic effect and the physics of waves. *American Journal of Physics*. 48(1). pp. 41–47. DOI: 10.1119/1.12250.
2. Schmid T. (2006) Photoacoustic spectroscopy for process analysis. *Analytical and Bioanalytical Chemistry*. 384(5). pp. 1071–1086. DOI: 10.1007/s00216-005-3281-6.
3. Davies S.J., Edwards C., Taylor G.S., Palmer S.B. (1993) Laser-generated ultrasound: its properties, mechanisms and multifarious applications. *Journal of Physics D: Applied Physics*. 26(3). pp. 329–348. DOI: 10.1088/0022-3727/26/3/001.
4. Hutchins D.A., Wilkins D.E. (1985) Elastic waveforms using laser generation and electromagnetic acoustic transducer detection. *Journal of Applied Physics*. 58. pp. 2469–2477. DOI: 10.1063/1.335923.
5. Nosaka Y., Igarashi R., Miyama H. (1985) Pulsed photoacoustic spectroscopy for powder suspension using a flash lamp. *Analytical Chemistry*. 57(1). pp. 92–94. DOI: 10.1021/ac00279a026.
6. Nelson E.T., Patel C.K.N. (1981) Response of piezoelectric transducers used in pulsed optoacoustic spectroscopy. *Optics Letters*. 6(7). pp. 354–356. DOI: 10.1364/OL.6.000354.
7. Rosencwaig A. (1975) Photoacoustic spectroscopy of solids. *Physics Today*. 28(9). pp. 23–30. DOI: 10.1063/1.3069155.
8. Rosencwaig A., Gersho A. (1976) Theory of the photoacoustic effect with solids. *Journal of Applied Physics*. 47(1). pp. 64–68. DOI: 10.1063/1.322296.
9. McDonald F., Wetsel G. (1978) Generalized theory of the photoacoustic effect. *Journal of Applied Physics*. 49(4). pp. 2313–2322. DOI: 10.1063/1.325116.
10. Quimby R., Yen W. (1980) Photoacoustic theory including energy migration. *Journal of Applied Physics*. 51(9). pp. 4985–4990. DOI: 10.1063/1.328377.
11. Chow H. (1980) Theory of three dimensional photoacoustic effect with solids. *Journal of Applied Physics*. 51(8). pp. 4053–4056. DOI: 10.1063/1.328255.
12. Merzadinova G., Sakipov K., Sharifov D., Mirzo A., Bekeshev A. (2019) Laser photoacoustics method for determination of the coefficients of thermal conductivity and thermal diffusivity of materials. *Eurasian Physical Technical Journal*. 16(1). pp. 94–98. DOI: 10.31489/2019No1/94-98.
13. Viator J.A., Jacques S.L., Prahl S.A. (1999) Depth profiling of absorbing soft materials using photoacoustic methods. *IEEE Journal of Selected Topics in Quantum Electronics*. 5(4). pp. 989–996. DOI: 10.1109/2944.796321.

14. Sigrist M.W. (1999) Photoacoustic spectroscopy, method and instrumentation. *Encyclopedia of Spectroscopy and Spectrometry*. 3. p. 1810.
15. Pincus R.L. (2014) Photoacoustic spectroscopy: a method for investigating weak molecular absorption. *Reed College Journal*. p. 43.
16. Bell A.G. (1880) Photoacoustic imaging and spectroscopy. *American Journal of Science*. 20. p. 305.
17. Haisch C., Niessner R. (2002) Light and sound – photoacoustic spectroscopy. *Spectroscopy Europe*. 14(5). pp. 10–15.
18. West G.A., Barrett J.J., Siebert D.R., Reddy K.V. (1983) Photoacoustic spectroscopy. *Review of Scientific Instruments*. 54. pp. 797–817. DOI: 10.1063/1.1137483.
19. White R.M. (1963) Generation of elastic waves by transient surface heating. *Journal of Applied Physics*. 34(12). pp. 3559–3567. DOI: 10.1063/1.1729258.
20. Salikhov T.Kh., Melikkhudzha N., Khodzhaev Y.P., Khodzhakhonov I.T. (2017) K teorii generatsii fotoakusticheskogo signala tverdotel'nymi obraztsami [To the theory of generation of photoacoustic signal by solid state samples]. *Doklady Akademii nauk Respubliki Tajikistan – Reports of the Academy of Sciences of the Republic of Tajikistan*. 60(11-12). pp. 569–574.
21. Nelson E.T., Patel C.K.N. (1981) Response of piezoelectric transducers used in pulsed opto-acoustic spectroscopy. *Optics Letters*. 6(7). pp. 354–356. DOI: 10.1364/OL.6.000354.
22. Scruby C.B., Wadley H.N.G. (1978) A calibrated capacitance transducer for the detection of acoustic emission. *Journal of Physics D: Applied Physics*. 11(1). pp. 1487–1494. DOI: 10.1088/0022-3727/11/11/007.
23. Sarode A.P., Mahajan O.H. (2018) Theoretical aspects of photoacoustic effect with solids. *International Journal for Science and Advance Research in Technology*. 4(2). pp. 1237–1242. DOI: 10.13140/RG.2.2.21345.45921.
24. Ailawalia P., Sachdeva S.K., Singh P.D. (2017) Effect of mechanical force along the interface of semi-infinite semiconducting medium and thermo-elastic micropolar cubic crystal. *Cogent Mathematics*. 4(1). pp. 231–234. DOI: 10.1080/23311835.2017.1347991.
25. Nyawere P.W.O., Makau N.W., Amolo G.O. (2014) First-principles calculations of the elastic constants of the cubic, orthorhombic and hexagonal phases of BaF_2. *Physica B: Condensed Matter*. 434. pp.122–128. DOI: 10.1016/j.physb.2013.10.051.
26. Mahmoud S.R., Ghaleb Sh.A., Alzahrani A.K., Ghandourah E. (2017) Mathematical model for problem of stresses in thermo-magneto-piezoelectric material. *Applied Mathematics & Information Sciences*. 11(4). pp. 1217–1223. DOI: 10.18576/amis/110429.
27. Patel S.R. (1971) Inverse problems of transient heat conduction with radiation. *The Mathematics Education*. 5(4). pp. 85–90.
28. Sneddon I.N. (1974) *The Use of Integral Transform*. New Delhi: Tata McGraw-Hill.

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