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Theoretical aspects of transient temperature on cubic crystal surface in a photoacoustic effect

In photoacoustic effect, the solid sample absorbs a fraction of the radiation falling upon it and excitation process occurs. The type of excitation depends on the energy of the incident radiation. The relaxation processes, which are also popularly known as non-radiative de-excitation processes generally take place. The light – matter interaction is responsible for the generation of heat within the solid sample. The temperature of the sample changes due to absorption and non-radiative relaxation by the atoms. The pressure fluctuations will be generated due to the heating and cooling of the sample. Today, crystalline solids are widely studied due to their wide scientific and industrial applications. Temperature is one of the important parameter to be studied regarding artificial preparation of large crystals. In this paper, transient translational temperature on the surface of a homogeneous isotropic cubic crystal kept in a photoacoustic cell is calculated theoretically. For a simple cubic homogeneous crystal kept in a photoacoustic cell, an airy stress function is determined based on laser interaction with surface of the crystal. By applying the finite Marchi-Fasulo integral transform method within the crystal size limitations, transient translational temperature is exactly determined.

Keywords: airy stress function, cubic crystal, energy transfer, light – matter interaction, Marchi-Fasulo transform, non-radiative de-excitation, photoacoustic cell, photoacoustic effect, transient temperature,

Introduction

Photoacoustic effect is a phenomenon in which electromagnetic radiation is absorbed by molecules of sample material. In 1880–1881, Alexander Graham Bell [1] found the interaction of light with solid. When mechanically chopped sunlight incident on a thin disk, sound waves were generated. This effect is called as Photoacoustic effect. The conversion of an optical signal into an acoustic signal takes place in photoacoustic effect [2]. The solid sample absorbs a fraction of the radiation falling upon it and excitation process occurs. The type of excitation depends on the energy of the incident radiation. The relaxation processes, which are also popularly known as non-radiative de-excitation processes generally, take place. The light – matter interaction is responsible for the generation of heat within the solid sample [3].

Rosencwaig initiated theoretical explanation of temperature of solids during photoacoustic interaction [4]. Rosencwaig and Gersho presented a one dimensional model regarding heat flow and temperature [5]. McDonald and Wetsel presented temperature calculations of photoacoustic interaction in three dimensional model with restrictions on thermal waves in transverse direction [2]. Quimby and Yen primarily calculated the surface heat conductance in temperature estimation [6]. Chow developed a three dimensional model in a general way without any restrictions on sample size in photoacoustic cell [7]. 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 [8].

In this paper, an attempt has been made to calculate transient translational temperature on the surface of a homogeneous isotropic cubic crystal kept in a photoacoustic cell. Determination of transient translational temperature will be helpful in the development of a methodology of stress determination in photoacoustic problems.

Situation of the crystal

Consider a cubic crystal placed in a photoacoustic cell. The crystal is isotropic and homogeneous in nature. This crystal is placed in a cylindrical cavity of a photoacoustic cell where it produces a photoacoustic signal.

The Photoacoustic effect is directly related with on heating of the sample due to the phenomenon of optical absorption [9, 10]. Periodic processes of heating and cooling of the solid sample are necessary because it will develop pressure fluctuations should be generated in the cell [11]. These fluctuations can be detected by a sensitive sensor.

In the schemes of modulated excitation, sources of radiation are used in which intensity periodically fluctuates [12–16]. These intensity fluctuations are in the form of a sine wave or a square wave. This is similar to mechanical chopping of a radiation source. This method can be overcome by modulating the phase of the optical signal instead of its amplitude [17–19]. The most common sources in Photoacostic analysis are the use of modulated continuous wave lasers.

Two level system model

To describe the absorption of light, consider a two level system, in which energy transfers take place, as shown in Figure 1. These energy transfers are radiative and non-radiative. Let us consider two states *i* and *j*. Also, consider the coefficients $\mathbf{r_{ij}}$ and $\mathbf{c_{ij}}$. The radiative transition rate is $\mathbf{r_{ij}}$ and non-radiative transition rate is $\mathbf{c_{ij}}$. The coefficient $\mathbf{c_{ij}}$ is also called collision-induced energy transfer. Now, introduce Einstein coefficients for stimulated and spontaneous emission, B_{ij} and A_{ij}. Consider that ρ_ω be the spectral energy density for the corresponding frequency of the transition between E_0 and E_6. Einstein coefficients can be expressed as

$$\mathbf{r_{ij}} = \rho_\omega \mathbf{B_{ij}} + \mathbf{A_{ij}} \quad (1)$$

The quantity ρ_ω measures the radiant energy per volume per unit frequency and can be expressed in terms of units JS/m^3.

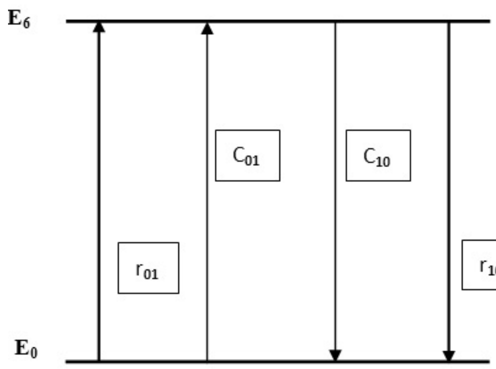

Figure 1. A schematic representation of a two level system

Note that $B_{ij} = B_{ji}$ so that $B_{06} = B_{60}$. But $A_{06} = 0$ because spontaneous emission from a state of lower energy to that of higher energy does not exist. Hence $r_{06} = \rho_\omega B_{06}$. Again, the probability of excitation due to collision from E_0 to E_6 is very low, Therefore, approximately we can say, $c_{06} \sim= 0$.

Let us determine the rate of transition. For this calculation, we must distinguish the population densities of absorbing molecules in the ground and excited states. Consider these population densities as n_0 and n_6, respectively corresponding to energies E_0 and E_6. To calculate the rate of change of population in upper state, we must consider the difference between the number of molecules entering and leaving the excited state:

$$\dot{n}_6 = (r_{06} + c_{06})n_0 - (r_{60} + c_{60})n_6$$

$$\dot{n}_6 = \rho_\omega B_{06}n_0 - (\rho_\omega B_{06} + A_{60} + c_{60})n_6$$

$$\dot{n}_6 = \rho_\omega B_{06}(n_0 - n_6) - (A_{60} + c_{60})n_6. \quad (2)$$

Let the radiative and collisional time constants be $\tau_r = 1/A_{60}$ and $\tau_c = 1/c_{60}$ respectively.

The total time constant is, then addition of radiative and collisional time constants:

$$\tau = \tau_r + \tau_c.$$

Mathematical formulation

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

$$\text{D: } -a \le x \le a\,,\ -a \le y \le a\ .\ -a \le z \le a\,.$$

Consider a Cartesian co-ordinate system, in which the displacement components are u_x, u_y, u_z in the x, y, z direction respectively. These displacement components can be expressed in the integral form as

$$u_x = \int \left[\frac{1}{Y}\left(\frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} - \nu \frac{\partial^2 U}{\partial x^2} \right) + \lambda T \right] dx\,; \tag{2.1}$$

$$u_y = \int \left[\frac{1}{Y}\left(\frac{\partial^2 U}{\partial z^2} + \frac{\partial^2 U}{\partial x^2} - \nu \frac{\partial^2 U}{\partial y^2} \right) + \lambda T \right] dy\,; \tag{2.2}$$

$$u_z = \int \left[\frac{1}{Y}\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} - \nu \frac{\partial^2 U}{\partial z^2} \right) + \lambda T \right] dz\,. \tag{2.3}$$

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. Consider that $U(x, y, z, t)$ is the Airy stress function which satisfies the differential equation.

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)^2 U(x,y,z,t) = -\lambda Y \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)^2 T(x,y,z,t)\,. \tag{2.4}$$

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

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} + \frac{\theta(x,y,z,t)}{k} = \frac{1}{\alpha}\frac{\partial T}{\partial t}\,, \tag{2.5}$$

where k is thermal conductivity and α is the thermal diffusivity of the material of the crystal.

Let $\theta(x,y,z,t)$ is heat generated within the crystal for $t > 0$ subject to initial conditions

$$T(x,y,z,0) = F(x,y,z)\,. \tag{2.6}$$

The boundary conditions are

$$\left[T(x,y,z,t) + k_1 \frac{\partial T(x,y,z,t)}{\partial x} \right]_{x=-a} = F_1(y,z,t)\,; \tag{2.7}$$

$$\left[T(x,y,z,t) + k_2 \frac{\partial T(x,y,z,t)}{\partial x} \right]_{x=a} = F_2(y,z,t)\,; \tag{2.8}$$

$$\left[T(x,y,z,t) + k_3 \frac{\partial T(x,y,z,t)}{\partial y} \right]_{y=-a} = F_3(x,z,t)\,; \tag{2.9}$$

$$\left[T(x,y,z,t) + k_4 \frac{\partial T(x,y,z,t)}{\partial y} \right]_{y=a} = F_4(x,z,t)\,; \tag{2.10}$$

$$\left[T(x,y,z,t) + k_5 \frac{\partial T(x,y,z,t)}{\partial z} \right]_{z=-a} = f_1(x,y,t)\,; \tag{2.11}$$

$$\left[T(x,y,z,t) + k_6 \frac{\partial T(x,y,z,t)}{\partial z} \right]_{z=a} = f_2(x,y,t)\,. \tag{2.12}$$

The components in term of $U(x, y, z, t)$ are given by

$$\sigma_{xx} = \left(\frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} \right); \tag{2.13}$$

$$\sigma_{yy}=\left(\frac{\partial^2 U}{\partial z^2}+\frac{\partial^2 U}{\partial x^2}\right); \tag{2.14}$$

$$\sigma_{zz}=\left(\frac{\partial^2 U}{\partial x^2}+\frac{\partial^2 U}{\partial y^2}\right). \tag{2.15}$$

The equations (2.1) to (2.15) constitute the mathematical formulation of the conditions of the crystal under consideration.

Mathematical solution

The finite Marchi-Fasulo integral transform of f (z), within limitations -h < z < h is defined to be

$$\bar{F}=\int_{-h}^{h} f(z)P_n(z)\,dz. \tag{3.1}$$

Then at each point of (–*h*, *h*) at which *f* (*z*) is continuous.

Also the inverse finite Marchi-Fasulo transform is defined as

$$f(z)=\sum_{n=1}^{\infty}\frac{\bar{F}(n)}{\lambda_n}P_n(z), \tag{3.2}$$

where

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

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

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

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

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

The Eigen values a_n are the solutions of the equation

$$\left[\alpha_1 a\cos(ah)+\beta_1\sin(ah)\right]\times\left[\beta_2\cos(ah)+\alpha_2 a\sin(ah)\right]=\left[\alpha_2 a\cos(ah)-\beta_2\sin(ah)\right]\times$$
$$\times\left[\beta_1\cos(\mathrm{ah})-\alpha_1\mathrm{a}\sin(\mathrm{ah})\right] \tag{3.3}$$

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

By applying the finite Marchi-Fasulo transform three times to equation (2.5) and their inverses, we obtain

$$\frac{d\,\bar{\bar{T}}^*}{dt}+\propto q^2\,\bar{\bar{T}}^*=\propto\left(\varnothing+\frac{\bar{\bar{\theta}}^*}{k}\right), \tag{3.4}$$

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 Eigen value. (3.5)

Equation (3.4) is first order differential equation and has solution

$$\bar{\bar{T}}^*(m,n,l,t)=e^{-\propto q^2 t}\left[\int_0^t\propto\left(\varnothing+\frac{\bar{\bar{\theta}}^*}{k}\right)e^{\propto q^2 t' dt'}+c\;\;,c=\bar{\bar{F}}^*(m,n,l)\right]; \tag{3.6}$$

$$\bar{\bar{T}}^*(m,n,l,t)=\int_0^t\propto\left(\varnothing+\frac{\bar{\bar{\theta}}^*}{k}\right)e^{\propto(a_m^{\;2}+a_n^{\;2}+a_l^{\;2})(t-t')dt'}+e^{-\propto(a_m^{\;2}+a_n^{\;2}+a_l^{\;2})t}\,\bar{\bar{F}}^*(m,n,l). \tag{3.7}$$

Applying inverse finite Marchi- Fasulo Transform three times with boundary conditions, we get

$$T(x,y,z,t)=\sum_{m,n,l=1}^{\infty}\left[\frac{P_m(x)}{\lambda_m}\right]\left[\frac{P_n(y)}{\mu_n}\right]\left[\frac{P_l(z)}{\nu_l}\right]\left\{\int_0^t \propto\left(\varnothing+\frac{\overset{=}{\theta}^*}{k}\right)e^{\propto(a_m^2+a_n^2+a_l^2)(t-t')dt'}+e^{-\propto(a_m^2+a_n^2+a_l^2)t}\,\overset{=}{F}^*(m,n,l)\right\}. \quad (3.8)$$

Conclusion

An exact expression for the transient translational temperature on the surface of a cubic crystal in a photoacoustic cell is mathematically determined using Marchi-Fasulo method in terms of thermal conductivity of material of the crystal.

The result obtained will be helpful in the study of cubic crystals, and their various properties such as elasticity, stress, strain, etc. in photoacoustic cell. The elastic parameters of the crystals are studied more than only academic interest. Crystals of better quality and large size are synthetically prepared in application point of view. Transient translational temperature determination will provide a base for surface behavior of crystals of different materials in laser interactions in Photoacoustic effect. This work will also be useful in research for scientific and industrial applications in future.

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А.П. Сарод, О.Х. Махаджан

Фотоакустикалық әсердегі текше кристалдың бетіндегі өтпелі температураның теориялық аспектілері

Фотоакустикалық әсер кезінде қатты үлгі оған түсетін сәулеленудің бір бөлігін жұтады және қозу процесі жүреді. Қозу түрі түскен сәулеленудің энергиясына байланысты. Түссізденудің радиациялық емес процестер ретінде де белгілі релаксация процестері өз орынын алады. Жарық пен заттың өзара әрекеттесуі қатты үлгінің ішінде жылу шығаруға жауап береді. Үлгінің температурасы атомдардың жұтылуына және радиациялық емес релаксациясына байланысты өзгереді. Қысымның ауытқуы үлгіні қыздыру мен салқындатуға байланысты пайда болады. Бүгінгі таңда кристалды қатты заттар олардың кең ғылыми және өнеркәсіптік қолданылуына байланысты кеңінен зерттелуде. Температура — үлкен кристалдарды жасанды түрде алу кезінде зерттелетін маңызды параметрлердің бірі. Жұмыста фотоакустикалық ұяшықта сақталатын біртекті изотропты текше кристалдың бетіндегі өтпелі аудармалы температура теориялық тұрғыдан есептелген. Фотоакустикалық ұяшықтағы қарапайым текше біртекті кристалл үшін кристалл бетімен лазерлік өзара әрекеттесуге негізделген Эйри кернеуінің функциясы анықталған. Марки-Фасулоның ақырғы интегралдық түрлендіру әдісін кристалл мөлшерінің шектеулері аясында қолдана отырып, өтпелі аударма температурасын дәл анықтауға болады.

Кілт сөздер: Эйри кернеуінің функциясы, текше кристалл, энергияны тасымалдау, жарық пен заттың өзара әрекеттесуі, Марчи-Фасулоның түрленуі, радиациялық емес қозу, фотоакустикалық жасуша, фотоакустикалық әсер, өтпелі температура.

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Теоретические аспекты переходной температуры на поверхности кубического кристалла в фотоакустическом эффекте

При фотоакустическом эффекте твердый образец поглощает часть падающего на него излучения и происходит процесс возбуждения. Тип возбуждения зависит от энергии падающего излучения. Релаксационные процессы, которые также широко известны как нерадиационные процессы высвечивания, обычно имеют место. Взаимодействие света и вещества ответственно за генерацию тепла внутри твердого образца. Температура образца подвергается изменению за счет поглощения и нерадиационной релаксации атомами. Колебания давления будут генерироваться из-за нагрева и охлаждения образца. Сегодня кристаллические твердые тела широко изучаются благодаря их широкому научному и промышленному применению. Температура является одним из важных параметров, подлежащих изучению при искусственном получении крупных кристаллов. В настоящей работе теоретически рассчитана переходная поступательная температура на поверхности однородного изотропного кубического кристалла, удерживаемого в фотоакустической ячейке. Для простого кубического однородного кристалла, содержащегося в фотоакустической ячейке, определяется функция напряжения Эйри, основанная на лазерном взаимодействии с поверхностью кристалла. Применяя метод конечных интегральных преобразований Марчи-Фасуло в рамках ограничений размера кристалла, можно точно определить переходную поступательную температуру.

Ключевые слова: функция напряжения Эйри, кубический кристалл, перенос энергии, взаимодействие света и вещества, преобразование Марчи-Фасуло, нерадиационное де-возбуждение, фотоакустическая ячейка, фотоакустический эффект, переходная температура.

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