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Displacement fields of a Cuboid crystal in a Photoacoustic Cell: Mathematical aspects

Photo acoustic effect is popular due to a minimal sample preparation during execution, the ability to examine scattering and opaque sample along with the capability to access depth profile. These features enable Photoacoustic spectroscopy to be used in depth-resolved characterization of solids. Thermal interaction is a basic perspective in solid state physics research regarding industrial devices and components. It is a key factor of fabrication and performance of such devices and components. Today, crystalline solids are widely studied due to their wide scientific and industrial applications. Displacement field resulting in thermal stresses is one of the important aspects of premature failure of industrial components and devices. In this paper, displacement fields in photoacoustic effect with solid cuboid crystal are mathematically presented. According to our opinion, displacement fields in photoacoustic effect in three dimensional analysis are not reported earlier. Hence that will be a major contribution of this paper. For a simple cuboid 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, displacement field is exactly determined.

Keywords: airy stress function, cuboid crystal, displacement field, energy transfer, light – matter interaction, Marchi- Fasulo transform, non-radiative de-excitation, photoacoustic cell, photoacoustic effect.

Introduction

A displacement field is a scalar function which enables us to determine different stresses in an elastic body by simple differentiation method. In this paper, an attempt has been made to calculate displacement fields of a homogeneous isotropic cubic crystal kept in a modified photoacoustic cell. Determination of displacement field will be helpful in the development of a methodology of application of displacement field to stress determination in photoacoustic problems.

When incident radiation is absorbed by molecules of the target material, photoacoustic effect is generated [1-2]. Photoacoustic effect can be used in depth-resolved thermal characterization of materials [3]. The interaction of incident radiation with the atoms of the material in the crystal results in the generation of heat [4]. This heat generation is applied to calculate displacement fields in the crystal. The Marchi-Fasulo integral transform method is used here to calculate displacement fields in an isotropic cuboid crystal in photoacoustic effect.

Initial theoretical explanation of temperature of solids during photoacoustic interaction was presented by Rosencwaig [5]. A one dimensional model regarding heat flow and temperature was formulated by Rosencwaig and Gersho [6]. McDonald and Wetsel published temperature calculations of photoacoustic interaction in three dimensional model with restrictions on thermal waves in transverse direction [7]. Quimby and Yen primarily calculated the surface heat conductance in temperature estimation [8]. Chow developed a three dimensional model in a general way without any restrictions on sample size in photoacoustic cell [9]. 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 [10].

Situation of the crystal

Consider a cuboid crystal placed in a photoacoustic cell. The crystal is isotropic and traction free in nature. This crystal is placed in a cylindrical cavity of a photoacoustic cell which produces a photoacoustic signal. The cell is air tight. Hence the cell has a constant volume of gas surrounding the crystal. The crystal is irradiated by a proper modulated laser source. The crystal absorbs heat and generates photoacoustic signal.

The Photoacoustic effect is directly related with on heating of the sample due to the phenomenon of optical absorption [11-12]. Periodic processes of heating and cooling of the solid sample are necessary because it will develop pressure fluctuations should be generated in the cell [13]. These fluctuations can be detected by a sensitive sensor.

In the process of modulated excitation, sources of radiation are used in which intensity fluctuates periodically [14-17]. These fluctuations in the intensity of radiation are in the form of a sine wave or a square wave. This is similar to mechanical chopping of a radiation source. To modulate the phase of the optical signal instead of its amplitude is the best way to overcome this method [18-20]. In Photoacostic analysis, the most common sources are the use of modulated continuous wave lasers.

Mathematical formulation

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

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

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

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

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

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

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,

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)^2 U(x,y,z,t) = -\lambda Y \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)^2 T(x,y,z,t) \tag{4}$$

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

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} + \frac{\theta(x,y,z,t)}{k} = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{5}$$

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 (5).

$$T(x,y,z,0) = F(x,y,z) \tag{6}$$

Boundary Conditions

Let us define boundary conditions on the crystal. These boundary conditions are

$$\left[\mathrm{T(x,y,z,t)} + \mathrm{k}_1 \frac{\partial T(x,y,z,t)}{\partial x}\right]_{x=a} = F_1\,(y,z,t) \tag{7}$$

$$\left[\mathrm{T(x,y,z,t)} + \mathrm{k}_2 \frac{\partial T(x,y,z,t)}{\partial x}\right]_{x=-a} = F_2\,(y,z,t) \tag{8}$$

$$\left[\mathrm{T(x,y,z,t)} \; + \mathrm{k}_3 \frac{\partial T(x,y,z,t)}{\partial y}\right]_{y=b} \quad = F_3\,(x,z,t) \tag{9}$$

$$\left[\mathrm{T(x,y,z,t)} \; + \mathrm{k}_4 \frac{\partial T(x,y,z,t)}{\partial y}\right]_{y=-b} \quad = F_4\,(x,z,t) \tag{10}$$

$$\left[\mathrm{T(x,y,z,t)} \; + \mathrm{k}_5 \frac{\partial T(x,y,z,t)}{\partial z}\right]_{z=0} \quad = \mathrm{f}_1\,(x,y,t) \tag{11}$$

$$\left[\mathrm{T(x,y,z,t)} \; + \mathrm{k}_6 \frac{\partial T(x,y,z,t)}{\partial z}\right]_{z=-h} \quad = \mathrm{f}_2\,(x,y,t) \tag{12}$$

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

$$\sigma_{xx} = \left(\frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2}\right) \tag{13}$$

$$\sigma_{yy} = \left(\frac{\partial^2 U}{\partial z^2} + \frac{\partial^2 U}{\partial x^2}\right) \tag{14}$$

$$\sigma_{zz} = \left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}\right) \tag{15}$$

The “Eq. (1)” to “(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

$$\bar{F} = \int_{-h}^{h} f(z)\, P_n(z)\, dz \tag{16}$$

Then at each point of *(-h, h)* , the function *f (z)* is continuous. Again, the inverse finite Marchi - Fasulo transform for previous conditions is defined as

$$f(z) = \sum_{n=1}^{\infty} \frac{\bar{F}(n)}{\lambda_n} P_n(z) \tag{17}$$

Here,

$$P_n(z) = Q_n \cos(a_n z) - W_n \sin(a_n z)$$
$$Q_n = a_n(\alpha_1 + \alpha_2)\cos(a_n h) + (\beta_1 - \beta_2)\sin(a_n h)$$
$$W_n = (\beta_1 + \beta_2)\cos(a_n h) + (\alpha_1 - \alpha_2) a_n \sin(a_n h)$$
$$\lambda_n = \int_{-h}^{h} {P_n}^2(z) dz$$
$$\lambda_n = h\left[{Q_n}^2 + {W_n}^2\right] + \frac{\sin(2a_n h)}{2a_n}\left[{Q_n}^2 - {W_n}^2\right]$$

The Eigen values a_n are the solutions of the equation

$$[\alpha_1 a\cos(ah) + \beta_1 \sin(ah)] \times [\beta_2 \cos(ah) + \alpha_2 a\sin(ah)] =$$
$$= [\alpha_2 a\cos(ah) - \beta_2 \sin(ah)] \times [\beta_1 \cos(ah) - \alpha_1 a\sin(ah)] \tag{18}$$

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

By applying the finite Marchi - Fasulo transform three times to “Eq. (5)” and their inverses, we obtain

$$\frac{d\bar{\bar{T}}^M}{dt} + \propto q^2 \bar{\bar{T}}^{*} = \propto \left(\emptyset + \frac{\bar{\theta}^M}{k}\right) \tag{19}$$

where

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

and

$$q^2 = a_m^2 + a_n^2 + a_l^2 \tag{20}$$

is Eigen value.

"Eq. (10)" is first order differential equation and has solution

$$\bar{\bar{T}}^{\ast}(m,n,l,t) = e^{-\propto q^2 t}\left[\int_0^t \propto (\emptyset + \frac{\bar{\theta}^M}{k})\right] e^{-\propto q^2 t' dt'} + c, c = \bar{\bar{F}}^{\ast}(m,n,l) \tag{21}$$

$$\bar{\bar{T}}^{\ast}(m,n,l,t) = \int_0^t \propto (\emptyset + \frac{\bar{\theta}^M}{k}) e^{\propto(a_m^2+a_n^2+a_l^2)(t-t')dt'} + e^{-\propto(a_m^2+a_n^2+a_l^2)t}\bar{\bar{F}}^{\ast}(m,n,l) \tag{22}$$

If we apply inverse finite Marchi - Fasulo Transform three times with boundary conditions to this equation, we get

$$T(x,y,z,t) = \frac{k}{c^2}\sum_{m,n=1}^{\infty}\left[\frac{P_m(x)}{\lambda_m}\right]\left[\frac{P_n(y)}{\mu_n}\right][\varphi_1(z)\psi_1(t) - \varphi_2(z)\psi_2(t)] +$$

$$\frac{2k\pi}{h^2}\sum_{l,m,n=1}^{\infty}\left[\frac{P_m(x)}{\lambda_m}\right]\left[\frac{P_n(y)}{\mu_n}\right]\left[\frac{l}{\cos l\pi}\right]\left[\frac{1}{1+cl\pi^2}\right][n_1(z)\psi_3(t) - -n_2(z)\psi_4(t)] \tag{23}$$

Substituting the value of T(x, y, z ,t) from "Eq. (23)" in the "Eq. (4)", the airy stress function can be obtained as

$$U(x,y,z,t) = \lambda Y\frac{k}{c^2}\sum_{m,n=1}^{\infty}\left[\frac{P_m(x)}{\lambda_m}\right]\left[\frac{P_n(y)}{\mu_n}\right]\left[\frac{\varphi_1(z)\psi_1(t)-\varphi_2(z)\psi_2(t)}{a_m^2+a_n^2+\left\{\frac{1}{c}\right\}^2}\right] +$$

$$\frac{2\lambda Yk\pi}{h^2}\sum_{l,m,n=1}^{\infty}\left[\frac{P_m(x)}{\lambda_m}\right]\left[\frac{P_n(y)}{\mu_n}\right]\left[\frac{l}{\cos l\pi}\right]\left[\frac{\eta_1(x)\psi_3(t)-\eta_2(z)\psi_4(t)}{a_m^2+a_n^2+\left\{\frac{\pi}{h}\right\}^2}\right] \tag{24}$$

Results

The displacement field along x direction is calculated as

$$u_x = \alpha\frac{k}{c^2}\sum_{n,l=1}^{\infty}\left[\frac{(k_1+k_2)\sin 2a_m a}{\lambda_m}\right]\left[\frac{P_n(y)}{\mu_n}\right](1+\nu)a_m^2\left[\frac{\varphi_1(z)\psi_1(t)-\varphi_2(z)\psi_2(t)}{a_m^2+a_n^2+\left\{\frac{1}{c}\right\}^2}\right] +$$

$$\frac{2\propto k\pi}{h^2}\sum_{l,m,n=1}^{\infty}\left[\frac{(k_1+k_2)\sin 2a_m a}{\lambda_m}\right]\left[\frac{P_n(y)}{\mu_n}\right]\left[\frac{l}{\cos l\pi}\right]\left[\frac{\eta_1(z)\psi_3(t)-\eta_2(z)\psi_4(t)}{1+\left\{\frac{l\pi}{h}\right\}^2}\right] \tag{24}$$

In the similar way, displacement fields in other directions could be determined.

Conclusion

The exact expression for displacement field of a cuboid crystal in a photoacoustic cell is determined. The expression allows the calculation of various parameters of cuboid crystals properties such as stress, strain, etc related with elasticity in photoacoustic cell. This mathematical approach constitutes an important step towards determination of various aspects of premature failure of industrial components and devices This work will be useful in research for scientific and industrial applications in future.

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А.П. Сароде, О.Х. Махаджан

Фотоакустикалық ұяшықтағы текше тәрізді кристалдың ығысу өрістері: математикалық аспектілер

Фотоакустикалық эффект үлгіні дайындаудың ең аз уақытына, шашыраңқы және мөлдір емес үлгіні зерттеуге және тереңдік профилінің қолжетімділігіне байланысты танымал. Бұл ерекшеліктер терең ажыратымдылықтағы қатты заттардың сипаттамаларын анықтау үшін фотоакустикалық спектроскопияны қолдануға мүмкіндік береді. Термиялық әсерлесу — өнеркәсіптік құрылғылар мен компоненттерге қатысты қатты дене физикасын зерттеудегі басты перспектива. Бұл осындай құрылғылар мен компоненттерді шығарудың және дайындаудың негізгі факторы. Бүгінгі таңда кристалды қатты заттар кең ғылыми және өнеркәсіптік қолданудың арқасында кеңінен зерттелуде. Жылу кернеуіне әкелетін ығысу өрісі өнеркәсіптік қондырғылар мен құрылғылардың мерзімінен бұрын істен шығуының маңызды аспектілерінің бірі болып табылады. Жұмыста қатты кубоидты кристалмен фотоакустикалық әсердегі ығысу өрістері математикалық түрде ұсынылған. Авторлардың ойынша үш өлшемді анализде фотоакустикалық әсер кезінде орын ауыстыру өрістері бұрын байқалмаған. Демек бұл нақты құжатқа негізгі үлес болады. Фотоакустикалық ұяшықта орналасқан қарапайым кубоидты біртекті кристалл үшін Эйри кернеу функциясы лазердің кристалл бетімен әрекеттесуі негізінде анықталады. Марчи-Фасулоның түпкілікті интегралдық түрлендіру әдісін кристалл өлшемінің шектеулері шегінде қолдана отырып, ығысу өрісі дәл айқындалған.

Кілт сөздер: Эйри кернеуінің функциясы, текше тәрізді кристалл, ығысу өрісі, энергияны беру, жарық пен заттың өзара әрекеттесуі, Марчи-Фасуло түрлендіруі, сәулеленбейтін қозу, фотоакустикалық ұяшық, фотоакустикалық әсер.

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Поля смещения кубовидного кристалла в фотоакустической ячейке: математические аспекты

Фотоакустический эффект популярен благодаря минимальной пробоподготовке во время выполнения возможности исследовать рассеивающийся и непрозрачный образец наряду с доступом к профилю глубины. Эти особенности позволяют применять фотоакустическую спектроскопию для определения характеристик твердых тел с глубинным разрешением. Тепловое взаимодействие является основной перспективой в исследованиях физики твердого тела, касающихся промышленных устройств и компонентов. Это ключевой фактор изготовления и производительности таких устройств и компонентов. Сегодня кристаллические твердые тела широко изучены благодаря их широкому научному и промышленному применению. Поле смещений, приводящее к термическим напряжениям, является одним из важных аспектов преждевременного выхода из строя промышленных узлов и устройств. В работе математически представлены поля смещений в фотоакустическом эффекте с твердым кубовидным кристаллом. По мнению авторов, поля смещения при фотоакустическом эффекте в трехмерном анализе ранее не наблюдались. Следовательно, это будет главным вкладом в настоящий документ. Для простого кубовидного однородного кристалла, находящегося в фотоакустической ячейке, функция напряжения Эйри определена на основе взаимодействия лазера с поверхностью кристалла. Применение метода конечного интегрального преобразования Марчи–Фасуло в пределах ограничений размера кристалла позволило точно вычислить поле смещения.

Ключевые слова: функция напряжения Эйри, кубовидный кристалл, поле смещения, перенос энергии, взаимодействие света и вещества, преобразование Марчи–Фасуло, безызлучательное возбуждение, фотоакустическая ячейка, фотоакустический эффект.