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Numerical modeling of thermoelastic generation of ultrasound by laser irradiation in the coupled thermoelasticity

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ABSTRACT

Laser-generation of ultrasound is investigated in the coupled dynamical thermoelasticity in the presented paper. The coupled heat conduction and wave equations are solved using finite differences. It is shown that the application of staggered grids in combination with explicit integration of the wave equation facilitates the decoupling of the solution and enables the application of a combination of implicit and explicit numerical integration techniques. The presented solution is applied to model the generation of ultrasound by a laser source in isotropic and transversely isotropic materials. The influence of the coupling of the generalized thermoelasticity is investigated and it will be shown, that for ultra high frequency waves (i.e. 100 GHz) generated by laser pulses with duration in the picosecond range, the thermal feedback becomes considerable leading to a strong attenuation of the longitudinal bulk wave. Moreover, the coupling leads to dispersion influencing the wave velocities at low frequencies. The numerical simulations are compared to theoretical results available in the literature. Wave fields generated by a line focused laser source are presented by the numerical model for isotropic and for transversely isotropic materials.

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1. Introduction

Experimental application of laser-generated ultrasound in solids has a long and successful history. It has been extensively used in experimental acoustics in the past decades since it enables contactless excitation of different elastic waves, such as bulk, surface or guided waves. In search of better understanding and optimization of the generation mechanism, the modeling by a thermoelastic source has attracted great attention from the very beginning of the experimental application. Thus, the generation process is described by the coupled heat and wave equations, whereby various coupling terms are taken into account. One of the earliest work [1] has introduced a point-source representation of the thermal expansion as the so-called surface center of expansion. The corresponding elastic problem was solved by a spatial–temporal integral transform. Similar solutions have been pursued also by later authors applying an equivalent dipole loading in a pure elastic problem [2] or investigating the influence of the thermal diffusion on the generated bulk longitudinal wave [3]. These solutions have been extended to layered media [4] and to line sources in isotropic and transversely isotropic media [5,6]. For such analytic solutions, however, certain simplifications are required, such as a step-like temperature rise with a point or line spatial distribution for the surface heating. In general cases with more realistic distributions of the heat flux the inverse integral transforms remain a great challenge and consequently numerical inversion techniques were pursued. This approach was applied to investigate epicentral waveforms in [3,7,8], the generation process by line focused sources [9] or the influence of the hyperbolic term in the heat conduction equation [10]. Simplifications in the numerical inversion techniques are, however, controversial [11]. An alternative way to solve this coupled problem is shown in [12,13] using the reciprocity theorem with applications to a half space and plates.

Within laser ultrasonics the coupling of the heat and wave equations is due to thermal expansion leading to a semi-coupled problem. In the generalized thermoelasticity, however, also the thermal feedback of the propagating stress pulses is included, hence, the problem becomes fully coupled and both thermal and elastic waves arise [14]. Moreover, the coupling of the two fields influences the elastic wave velocities leading to additional dispersion and strong attenuation of the waves in isotropic [15,16] or in anisotropic media [17,18]. Although, the influence of the coupling on the wave velocity remains limited [15] the attenuation of pulses increases with frequency and it will be shown, that for laser pulses with duration of picoseconds or less the excited waves posses ultra high frequencies ($\sim$100 GHz) whereby this attenuation becomes considerable.

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Numerical methods, such as finite elements or finite differences have been rarely pursued to model laser-generation, though they offer a greater flexibility in their applications. A combination of an implicit-explicit finite difference technique has been applied in the one dimensional case to investigate the generation of bulk longitudinal waves [19] using the so-called magic time step [20]. The laser-generation of surface waves and bulk waves in coated and uncoated half spaces have been investigated using the finite element method in [21,22]. This solution applies a direct integration technique, though, the transient response could also be obtained by a combination of an Eigenvalue decomposition of the homogeneous equation and a harmonic analysis with an inverse Fourier-transform [23]. Numerical solutions are also capable to introduce full coupling as it was shown in [24] where a time domain finite element method was applied to study second sound effects due to heat propagation.

In the presented work laser-generation of ultrasound is investigated in the coupled dynamical thermoelasticity. In the presented numerical solution with staggered grids the two sets of equations decouple and therefore a combination of implicit and explicit finite difference techniques are applied. The hyperbolic heat conduction equation is solved by the implicit Wilson Θ integration technique and the wave equations by the explicit Euler method. Due to the combination of implicit and explicit techniques the same spatial and temporal discretisation are used for both sets of equations whereby the numerical efficiency remains high through the application of the explicit integration for the wave equation. The influence of coupling is investigated for line-focused pulsed laser sources with various pulse rise times. It will be shown, that for ultra high frequency waves ($\sim$100 GHz) the thermal feedback becomes considerable through strong attenuation. Moreover, the coupling increases the wave velocities for lower frequencies by introducing dispersion. Wave fields generated by the line focused laser source are presented by the numerical model for isotropic and also for transversely isotropic materials.

2. Governing equations

The governing equations of the generalized thermoelasticity in the linear elastic case are given by the coupled heat conduction and wave equations describing the coupling of displacement and temperature fields. In the presented work a 2D case with plane-strain boundary conditions is investigated, which is a good approximation of a line-focused laser source [9]. The hyperbolic heat conduction equation is given as:

$$K\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)=\rho c_v(\dot{T}+\tau\ddot{T})+T_0\beta_{xx}(\dot{\varepsilon}_{xx}+\tau\ddot{\varepsilon}_{xx}) + T_0\beta_{yy}(\dot{\varepsilon}_{yy}+\tau\ddot{\varepsilon}_{yy})-q, \quad (1)$$

where T denotes the temperatures, K the thermal conductivity, c_v the specific heat of the material at constant deformation, τ the material relaxation time, T_0 the reference temperature, q the external heat flux, ρ the density, $\varepsilon_{xx}, \varepsilon_{yy}$ the normal strains and β_{xx}, β_{yy} the thermal moduli. The wave equations are given as:

$$\rho\ddot{u}_x=\frac{\partial\sigma_{xx}}{\partial x}+\frac{\partial\sigma_{xy}}{\partial y}, \quad (2)$$

$$\rho\ddot{u}_y=\frac{\partial\sigma_{xy}}{\partial x}+\frac{\partial\sigma_{yy}}{\partial y}, \quad (3)$$

where u_x, u_y denotes the displacement components and $\sigma_{xx}, \sigma_{yy}, \sigma_{xy}$ are the stress components. In the presented work we consider an orthotropic material law with nine independent elastic constants and Hooke's law is replaced by the Duhamel–Neumann equations [25, p. 421–422] for the linear elasticity, which considers the effect of thermal expansion:

$$\sigma_{xx}=C_{11}\frac{\partial u_x}{\partial x}+C_{12}\frac{\partial u_y}{\partial y}-\beta_{xx}T, \quad (4)$$

$$\sigma_{yy}=C_{12}\frac{\partial u_x}{\partial x}+C_{22}\frac{\partial u_y}{\partial y}-\beta_{yy}T, \quad (5)$$

$$\sigma_{xy}=C_{44}\left(\frac{\partial u_x}{\partial y}+\frac{\partial u_y}{\partial x}\right). \quad (6)$$

According to the assumed orthotropy, the linear thermal expansion is described by three independent constants $\alpha_{xx}, \alpha_{yy}, \alpha_{zz}$ with three independent thermal moduli $\beta_{xx}, \beta_{yy}, \beta_{zz}$ [26, p. 25–26]. The thermal moduli $\beta_{xx}, \beta_{yy}, \beta_{zz}$ relate the stiffness matrix and the linear thermal expansion coefficients $\alpha_{xx}, \alpha_{yy}, \alpha_{zz}$ as:

$$\begin{aligned}\beta_{xx}&=C_{11}\alpha_{xx}+C_{12}\alpha_{yy}+C_{13}\alpha_{zz},\\ \beta_{yy}&=C_{12}\alpha_{xx}+C_{22}\alpha_{yy}+C_{23}\alpha_{zz},\\ \beta_{zz}&=C_{13}\alpha_{xx}+C_{23}\alpha_{yy}+C_{33}\alpha_{zz}.\end{aligned} \quad (7)$$

The heat conduction equation in Eq. (1) is given with its hyperbolic form, which assumes a finite heat propagation speed c_e, commonly approximated as five to ten times the longitudinal wave velocity c_l [9,10]. Here, we will assume that $c_e = 5c_l$ which leads to the following thermal relaxation time [10]:

$$\tau=\frac{K}{\rho c_v c_e^2}=\frac{K}{25\rho c_v c_l^2}. \quad (8)$$

Although the hyperbolic term in the presented heat equation becomes significant only for laser heating with duration in the fs–ps range, the validity of this equation for such ultrashort heating has been questioned [27]. During the heating process the free electrons absorb the radiated energy leading to a subsequent heating of the metal lattice through collisions. This non-equilibrium heating process is described by the two-temperature model [27] which assigns different temperatures to the electrons and to the lattice. According to previous results [19,27] this effect becomes significant for heating shorter than 1 ps (assuming room temperatures). To avoid implications by this effect we will restrict our investigations to cases where the laser heating is significantly longer than 1 ps; hence, the shortest pulse duration considered in the following is 20 ps.

2.1. Explicit–implicit finite difference approximation of the coupled equations

The spatial discretisation of the two sets of equations in Eqs. (1)–(6) is done with finite differences using staggered grids. Hence, the temperature, displacement and stress components are discretised on different grids which are shifted by a half cell in one or in both directions, according to Fig. 1. The grids of the temperatures and normal stresses are identical and the grids of the displacements and shear stresses are shifted by a half grid dimension ($\Delta x/2, \Delta y/2$).

The presented form of the coupled equations with stresses as additional variables (heterogenous solution [28,29]) is extensively applied in numerical solutions [19,30,31] since it requires only the first spatial derivatives to be discretised in the wave equation. The heterogenous, staggered grid formulism leads to further advantages in the investigated case due to decoupling of the discretised solution, as will be discussed later. Further details of discretisation with finite differences on staggered grids are not presented here, they can be found in [30–32], for example. Stress free boundary conditions to the wave equations and adiabatic boundary condition to the heat conduction equation are applied [19] and due to

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