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Modeling the distribution of phonon density for designing high quality thermal resonators

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ABSTRACT

An accurate theoretical model that quantifies the distribution of phonon density is indispensable for designing thermal resonators with high quality factor. This paper focuses on the modeling aspects of a generic cantilever structure excited thermally at resonance by applying Cattaneo-Vernotte hyperbolic heat conduction model. Critical analysis of the theoretical results revealed that the dynamic temperature oscillations at resonant frequencies are quantised wave responses whose characteristics ascribe to the quantum-mechanical behaviour of a particle inside a box. The theoretical predictions agree well with the experimental evaluation of the dynamic response of Al-Si_XN_Y bimaterial cantilever structure excited electrothermally by a signal with constant power spectral density. An increase in Q by a factor of 4–5 was achieved either by increasing the resonant frequency for a given length scale or by decreasing the length scale when excited by a signal with a constant power spectral density. This will enable to design micro/nano scale resonant devices with improved performance.

1. Introduction

Thermal excitation is very promising for realising high frequency resonators with large dynamic amplitude. The potential of thermal excitation have not been fully explored due to the lack of accurate theoretical models, which describe the heat transfer mechanisms at small scales. The mechanisms associated with the resonant energy transfer at different spatio-temporal intervals had been studied previously using different models namely, the Lattice-Boltzmann (LB) model [1], hyperbolic heat conduction (HHC) model proposed by Cattaneo-Vernotte (CV) [2] and Langevin model [3]. Recently, a unified theoretical formulation based on classical Fourier solution [4] showed enough evidence on the influence of phonon density in exciting the resonant modes of a structure thermally besides providing an in-depth physical insight on the underlying mechanisms. However quantifying the phonon density dictated by the interplay between length scale, material properties and frequencies have not been attempted yet for engineering high Q resonators driven thermally. In this light, the present work correlates the theoretical predictions with appropriate experimental data in order to establish the design guidelines. Practical applications include: resonant inertial sensors [5], mass sensors [6] and flow control resonant actuators.

The present study applies hyperbolic heat conduction (HHC) model proposed by Cattaneo-Vernotte for describing thermally driven resonant phenomenon. The suitability of HHC model based on equilibrium thermodynamics at time scales less than diffusion time is debatable. However, for most micro/nano-system devices with length scales varying between $\sim 10^{-1}$–10^{3} μm, this modeling approach provides a reasonably good estimates of temperature amplitude for interpreting the characteristics of thermal wave propagation. The physical significance of thermomechanical resonance was illustrated by critically analysing the effect of different parameters, which governs the dynamic temperature amplitude at resonance. The key objectives are: to evolve a suitable theoretical model for describing thermally driven resonant behaviour of cantilever structures and to corroborate theoretical predictions with relevant experimental data. Due consideration is given to the effect of spatial and temporal (frequency) variation on the Q-factor of the response when excited electrothermally by a signal with a constant power spectral density (PSD).

This paper is organised as follows. Section 2 discusses a theoretical model evolved using HHC solution. Section 3 discusses the physical significance of thermally driven resonant phenomenon by analysing the dynamic temperature amplitude. Section 4 discusses the design implications of the analytical model supplemented by experimental data. Section 5 draws the key concluding remarks from the present study.

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2. Analytical model for thermomechanical resonant excitation of a cantilever structure

The thermomechanical resonant condition is governed by the diffusion kinetics, which is dictated by the geometry, material properties, frequency of the forcing function and the thermal/mechanical boundary conditions [4]. At length/time scales associated with the mean free path of phonons, the diffusion phenomenon degenerates in to a thermal wave propagation phenomenon thereby causing spatial and temporal lag in the temperature gradient with respect to the heat flux vector [7]. The time scale for such a behaviour is of the order of thermal relaxation time, $\tau = 1/\omega_{th} \sim \alpha/c_{ph}^2$, where α is thermal diffusivity, $c_{ph} = c/\sqrt{3}$ is the phonon speed which is $(1/\sqrt{3})$ of the speed of sound, c for an isotropic material and ω_{th} is the threshold frequency above which heat transfer occurs by thermal wave propagation. Consider a cantilever beam of length, L with the fixed end at $x = 0$ as shown in Fig. 1. The flexural modes of the beam are excited thermally using a uniformly distributed harmonic heat generation source, $S = s_o e^{j\Omega t}$ where Ω is a constant excitation frequency. A one dimensional HHC thermal model for temperature prediction is given as [7]

$$\kappa A \frac{\partial^2}{\partial x^2} T(x,t) dx + A dx \left(S + \tau \frac{\partial S}{\partial t} \right) = \rho C A dx \left(\frac{\partial}{\partial t} + \tau \frac{\partial^2}{\partial t^2} \right) T(x,t) \quad (1)$$

where κ, C, ρ denote thermal conductivity, specific heat capacity, and density of the beam material. $T(x,t)$ represents temperature function at different spatial and temporal values. The geometry of the beam is defined by its length, L and its cross sectional area, A. The thermal boundary conditions for the problem defined by (1) is given as

$$(a)\ T(0,t) = T_w; \quad (b)\ T_x(L,t) = 0; \quad (c)\ T(x,0) = \phi_1(x); \quad (d)\ T_t(x,0) = \phi_2(x) \quad (2)$$

where T_w is the constant temperature heat sink at which the wall of the cantilever is maintained. The tip of the beam is thermally insulated due to high surface to volume ratio of most thin film structures [8]. Neglecting the higher order terms ($O(D^3)$ and $O(D^5)$) equation (1) can be rewritten as

$$\kappa \Theta_{xx} + (S + \tau S_t) = \rho C (\Theta_t + \tau \Theta_{tt}) \quad (3)$$

where $\Theta = T - T_W$. The suffixes x and t in (4) represents partial derivatives of T with respect to spatial and temporal variables respectively. The modified thermal boundary conditions associated with (3) are given as

$$(a)\ \Theta(0,t) = 0; \quad (b)\Theta_x(L,t) = 0; \quad (c)\Theta(x,0) = \phi(x) - T_w; \quad (d)\Theta_t(x,0) = \psi(x) - T_W \quad (4)$$

A general solution for the temperature field of the form

$$\Theta(x,t) = \sin(\beta x)\theta(t) \quad (5)$$

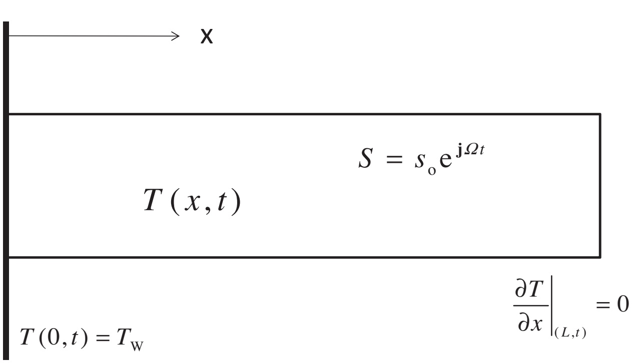

Fig. 1. Schematic of a cantilever beam subjected to periodic thermal excitation.

can be assumed which automatically satisfies (4a). Substituting (4b) in (5) leads to

$$\Theta(x,t) = \sin(\beta_m x)\theta_m(t) \quad (6)$$

where $\beta_m = (2m-1)\pi/2L$ and $m = 1,2,3,\ldots$ are harmonics of Fourier series. Rewriting the source term, S and the initial conditions, $\phi_1(x)$ and $\phi_2(x)$ as functions of Fourier harmonics, m gives

$$S = s_o e^{j\Omega t} = s_o D_m \sin(\beta_m x) e^{j\Omega t}; \quad \phi_1(x) = \phi_{1m}\sin(\beta_m x); \quad \phi_2(x) = \phi_{2m}\sin(\beta_m x) \quad (7)$$

where

$$D_m = \frac{2}{L}\int_0^L \sin(\beta_m x)dx; \quad \phi_{1m} = \frac{2}{L}\int_0^L \phi_1(x)\sin(\beta_m x)dx; \quad \phi_{2m} = \frac{2}{L}\int_0^L \phi_2(x)\sin(\beta_m x)dx \quad (8)$$

Substituting (7) in (3) and simplifying gives

$$\ddot{\theta}_m + \frac{\dot{\theta}_m}{\tau} + \frac{\beta_m^2 \alpha \theta_m}{\tau} = \frac{4 s_o (1 + j\Omega\tau) e^{j\Omega t}}{(2m-1)\pi\rho C\tau} \quad (9)$$

where $j = \sqrt{-1}$ is the imaginary unit of a complex number. Solution to equation (9) is given as

$$\theta_m(t) = e^{-t\omega_{th}/2}(C_1\cos(\omega'_{mt}t) + C_2\sin(\omega'_{mt}t)) + \frac{(1+j\Omega\tau)e^{j\Omega t}}{(\omega_{mt}^2 - \Omega^2) + j(1/4\tau^2)}\left(\frac{4 s_o \alpha}{(2m-1)\pi\kappa\tau}\right) \quad (10)$$

where $\alpha = \kappa/\rho C; \omega_{mt}^2 = (\beta_m^2 \alpha/\tau)$ and $\omega'_{mt} = (\sqrt{\omega_{mt}^2 - (1/4\tau^2)})$. The constants C_1 and C_2 can be obtained using the initial thermal boundary conditions given by (4c–d). However, for harmonic solution ($t \to \infty$), the exponential term, $e^{-t\omega_{th}/2}$ becomes zero and hence the constants C_1 and C_2 can be ignored. The harmonic response for a thermo-mechanical excitation can therefore be given as

$$\Theta(x,t) = \frac{(\omega_{th} + j\Omega)e^{j\Omega t}}{(\omega_{mt}^2 - \Omega^2) + j(\Omega\omega_{th})}\left(\frac{4 s_o \alpha}{(2m-1)\pi\kappa}\right)\sin(\beta_m x) \quad (11)$$

Critical examination of (11) reveals that the achievable temperature amplitude for a constant value of s_o increases with decreasing values of m which correspond to resonance. When Ω is equal to the natural frequency, ω_n of the structure, the magnitude of $\Theta(x, t)$ reaches maximum and hence $(\partial/\partial\Omega)(|\Theta(x,t)|) = 0$. Applying this condition along with $\Omega = \omega_n > 0$ leads to

$$m_{th} > \frac{L c_{ph}}{\pi\alpha}\sqrt{\sqrt{2} - 1} + \frac{1}{2} \quad (12)$$

where m_{th} is the threshold value of the Fourier harmonic to achieve resonance. It is evident from (12) that the Fourier harmonic, m at which resonance occurs (i.e. the energy required to excite the resonant modes) can be reduced by decreasing the resonant frequency and by increasing the thermal diffusivity of the material chosen. If S is a periodic chirp function ($S = s_o e^{j\sin[\Omega(t).t]}$ where $\Omega(t)$ is a chirp function), all resonant frequencies of the system within the chosen bandwidth will be excited at a constant energy. This causes the amplitude of vibration to drop with increasing values of ω_n within the chosen bandwidth.

3. Physical significance of thermomechanical resonance

Since temperature oscillations at resonance are thermoelastically transducted to mechanical velocity response, it is essential to achieve large amplitude of $\Theta(x, t)$ for small values of s_o. Perhaps a better insight on the physical mechanisms associated with thermally driven resonance can be obtained by analysing (11) applying quantum mechanics. At thermomechanical resonance, $\Omega = \omega_{mt} = \omega_n$, (11) reduces to