ICSV13 - Vienna
The Thirteenth International Congress on Sound and Vibration
Vienna, Austria, July 2-6, 2006

QUANTUM NONDESTRUCTIVE TESTING

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Abstract

Due to the arrival of nanotechnology which requires measurement up to the nanometer scale, and the interpretation of nanoscale/atomic scale phenomena using quantum mechanics, we propose the new field of quantum nondestructive testing which can be used for the nondestructive characterization of opaque nanometric multilayers and other nanostructures. Recently it has been demonstrated the generation of nanometer wavelength and THz frequency acoustic waves in strained piezoelectric layers induced by femtosecond optical pulses. The optically generated nano-acoustic wave (NAW) is then applied to one dimensional ultrasonic scan for thickness measurement which is the first step towards multi-dimensional nano-ultrasonic imaging. In this paper, we extend this optical piezoelectric transducer (OPT) technology to 2D nano-ultrasonic imaging with applications to nondestructive testing and medical imaging. We derive the expression for the scattered object wave using a microscopic theory based on quantum mechanics.

INTRODUCTION

Due to the arrival of nanotechnology, which requires measurement up to the nanoscale, and the interpretation of nanoscale/atomic scale phenomena using quantum mechanics, we propose the new field of quantum nondestructive testing, which can be used for the nondestructive characterization of opaque nanometric multilayers and other nanostructures. Picosecond ultrasonics [1] is a useful technique for analyzing the elastic and thermal properties of thin films, multilayers and nanostructures. It already has been applied to the nondestructive evaluation of opaque multilayered samples [2]. Metal film evaluation tools that measure the thickness of up to six layers in a multilayer metal film stack on 300mm product wafers are already commercialized (Rudolph Technologies, Inc. Flanders, NJ). Recently it has been demonstrated the generation of nanometer wavelength and THz frequency acoustic waves in strained piezoelectric layers induced by femtosecond optical pulses. The optically generated nano-acoustic wave (NAW) is then applied to one dimensional ultrasonic scan for thickness measurement which is the first step towards two-dimensional nano-ultrasonic imaging. This marks the beginning of the new field of nano-ultrasonics [3]. It has the capability of generating higher frequencies and better resolution than pico-ultrasound which can generate up to only around 300GHz. The femtosecond ultrasound technology is more advanced than the picosecond ultrasound technology.

MICROSCOPIC THEORY

The microscopic theory will be used because the thickness of the strained layers is only on the order of several nanometers. The piezoelectric InGaN/GaN multiple strained layers are used as the nano-structured optical piezoelectric transducer (OPT) for the generation of NAW. The cap layers of InGaN and GaN is the studied propagating medium.

To generate acoustic waves with a several nanometer wavelength, the thickness of the acoustic layer with a spatially modulated electric field distribution also should be on the order of several nanometers. It can be achieved easily with the matured epitaxial technology. However, for generating acoustic waves with a frequency in sub-terahertz to terahertz regime, the time to change the electric field should be less than 1ps. To achieve this requirement, a femtosecond (fs) optical pulse will provide the ultra high frequency initiating source.

Although the pulse width of the acoustic wave is on the scale of picoseconds, this technology still is unable to manipulate the phase of the initiated acoustic wave. However,terahertz coherent longitudinal-acoustic (LA) phonon oscillation generated in piezoelectric semiconductor multiple strained-layer structure (such as multiple quantum wells) was recently demonstrated. [4],[5] and a microscopic theory was presented later [6]. Because the wavelength of the acoustic wave is determined by the period of strained layers, it easily can be much less than 10nm. Because the acoustic wave is primarily induced through the piezoelectric effect, this multiple strained-layer structure (SLS) can be treated as an optical piezoelectric transducer (OPT) to generate nano-acoustic waves (NAW). Compared with a typical electrical transducer, the main difference is that the variation of the electric field in the nano-SLS OPT is induced by femtosecond laser pulses instead of electric pulses.

The following is a brief outline of the microscopic theory [6] for coherent acoustic phonon generation in super lattices and multiple quantum wells, including the effects of (i) band structure, (ii) strain, (iii) piezoelectric field, (iv) Coulomb interactions and (v) laser optical excitation.

In bulk systems, the conduction and valence bands in Wuertzite crystals including the effects of strain are treated using effective - mass theory. Near the band edge, the effective mass Hamiltonian for electrons is described by a 2×2 matrix that depends explicitly on electron wave vector K and the strain tensor ϵ. The electron Block basis states are taken to be

$$|C,1\rangle = |S\uparrow\rangle \tag{1a}$$

$$|C,2\rangle = |S\downarrow\rangle \tag{1b}$$

The conduction band Hamiltonian is diagonal and we have (relative to the bottom of the conduction band)

$$H^c_{2\times 2}(\underline{K},\underline{\epsilon}) = \left\{ \frac{\hbar^2 K_z^2}{2m_z^*} + \frac{\hbar^2 K_{yt}^2}{2m_{x-y}^*} + a_{c,z}\epsilon_{z,z} + a_{c,x-y}\epsilon_{z,z}(\epsilon_{x-x}+\epsilon_{y-y}) \right\} \mathrm{I}_{2\times 2} \tag{2}$$

where $\mathrm{I}_{2\times 2}$ is the identity matrix. The electron effective masses along z. The electron effective masses along z (taken to be parallel to the c axis) and in the $x-y$ plane are m_z^* and m_{x-y}^*, respectively. $K_t^2 = K_x^2 + K_y^2$ and ϵ_{x-x}, ϵ_{y-y} and ϵ_{z-z} are strain tensor components and $a_{c,z}$ and $a_{c,x-y}$ are the deformation potentials.

The second quantized Hamiltonian for electrons moving freely in the MQW interacting via a screened Coulomb potential. Denoting creation and destruction operators for electrons in conduction and valence subbands by $C^+_{\alpha,n,\underline{\mathbf{K}}}$ and $C_{\alpha,n,\underline{\mathbf{K}}}$, respectively, the second quantization Hamiltonian for free electrons and holes is simply:

$$\mathcal{H}_{eo} = \sum_{\alpha,n,\mathbf{K}} E_n^\alpha(K) C^+_{\alpha,n,\underline{\mathbf{K}}} C_{\alpha,n,\mathbf{K}} \tag{3}$$

The coherent phonon amplitude of the qth phonon mode $|q\rangle$ is defined to be [6]

$$D_q(t) = \langle b_q^+(t) + b_{-q}(t)\rangle \tag{4}$$

The coherent phonon amplitude is related to the macroscopic lattice displacement $U(z,t)$ and velocity $V(z,t)$ through the relations

$$U(z,t) = \sum_q \sqrt{\frac{\hbar^2}{2\rho_o(\hbar\omega_q)V}}\; e^{iqz} D_q(t) \tag{5}$$

$$V(z,t) = \sum_q \sqrt{\frac{\hbar^2}{2\rho_o(\hbar\omega_q)V}}\; e^{iqz} \frac{\partial D_q(t)}{\partial t} \tag{6}$$

The coherent phonon amplitude $D_q(t)$ will vanish if there are definite number of phonons in the mode i.e. if the phonon oscillator is in one of its energy eigenstates, $|q\rangle$. In this case there is no macroscopic displacement of the lattice.

The coherent phonon amplitudes $D_q(t)$ satisfy the driven harmonic oscillator equations

$$\frac{\partial^2 D_q(t)}{\partial t^2} + \omega_q^2 D_q(t) = -\frac{2\omega_q}{\hbar} \sum_{a,n,n',\mathbf{K}} M^\alpha_{n,n'}(K,q)^* \times \left\{ N^{\alpha,\alpha}_{n,n'}(K,t) - \delta_{\alpha,V}\delta_{n,n'} \right\} \tag{7}$$

subject to the initial conditions

$$D_q(t=-\infty) = \frac{\partial D_q(t=-\infty)}{\partial t} = 0 \tag{8}$$

By discretizing K and q and solving for $D(q_i)$ for each of the mesh points K_i and q_i, the resulting initial value ODE problem can be solved using a standard adaptive-step-size Runge-Kutta routine.

LOADED-STRING MODEL

The microscopic equations are rather detailed. They can be simplified (under certain conditions) to a more tractable model, namely, that of a driven uniform string, provided one uses the appropriate driving function $S(z,t)$, which is nonuniform. The microscopics, including details of the superlattice band structure and photogeneration process are included within the driving function.

In the detailed numerical simulations, the full microscopic formulation discussed previously will be used. A lot of insight can be obtained if we were to deal with the lattice displacement $U(z,t)$ directly. Assuming that the acoustic phonon dispersion relation is linear as follows:

$$\omega_q = C_S|q| = \sqrt{\frac{C_{33}}{\rho_o}}|q| \tag{9}$$

where ρ_o is the mass density and C_S is just the LA phonon sound speed for propagation parallel to $\hat{z}$ will satisfy the following loaded-string equation:

$$\frac{\partial^2 U}{\partial t^2}(z,t) - C_S^2\frac{\partial^2 U(z,t)}{\partial z^2} = S(z,t) \tag{10}$$

subject to the initial conditions

$$U(z,t=-\infty) = \frac{\partial U(z,t=-\infty)}{\partial t} = 0 \tag{11}$$

The LA sound speed C_S is defined in (9) and the driving function is given by

$$S(z,t) = -\frac{1}{\hbar}\sum_{a,n,n'}\sum_{\mathrm{K},q}\sqrt{\frac{2\hbar C_S|q|}{\rho_o V}}M^{\alpha}_{n',n}(K,q)^* \times \left\{N^{\alpha,\alpha'}_{n,n'}(K,t) - \delta_{\alpha,V}\delta_{n,n'}\right\}e^{iqz} \tag{12}$$

EXTENSION TO TWO DIMENSION CASE

In the nondestructive testing application, the above treatment will be extended to the two dimension case for 2D imaging. The loaded-string equation of (10) will become

$$\frac{\partial^2 U(r,t)}{\partial t^2} - C_S\frac{\partial^2 U(r,t)}{\partial r^2} = S(r,t) \tag{13}$$

subject to the initial conditions

$$U(r,t=-\infty) = \frac{\partial U(r,t=-\infty)}{\partial t} = 0 \tag{14}$$

and the driving function $S(r,t)$ will be given by

$$S(r,t) = -\frac{1}{\hbar} \sum_{a,n,n'} \sum_{\mathrm{K},q} \sqrt{\frac{2\hbar C_S |q|}{\rho_o V}} M^{\alpha}_{n',n}(K,q)^* \times \left\{ N^{\alpha,\alpha'}_{n,n'}(K,t) - \delta_{\alpha,V}\delta_{n,n'} \right\} e^{iqr} \quad (15)$$

POINTS TO BE CONSIDERED IN NONDESTRUCTIVE TESTING IMAGING

Spatial resolution

Because the time resolution of the optical detection is determined by the optical probe pulse width, not only high speed but also high spatial resolution can be achieved. For example, with an optical probe, pulse width of 100fs and an acoustic velocity of 8000m/s, the spatial resolution is better than 0.8nm. As for the detection of thin multilayers, the actual spatial resolution also is restricted by the acoustic wavelength and the acoustic pulse width. By resolving the envelope of the reflected acoustic echo, NAW easily can provide a spatial resolution down to several nanometers. By resolving the phase information and the interference between different echoes due to multilayers, a spatial resolution down to several angstroms is possible.

Optically determined acoustic beam size

The acoustic beam size of this technology is determined by the spot size of the excitation optical pulses. The cross-section area of the OPT thus can be tuned by controlling the illuminating area. If the diameter of the focused optical spot size is about 10 μm, then the generated NAW should be treated as plane waves. To further reduce the spot size, high numerical-aperture objective lens can achieve $<$ 200nm diameter focused spot-size at an ultraviolet optical wavelength. At the same time, NAW can be generated at arbitrary positions on the plane normal to the growth direction, controlled by the optical focal positions. This could be a powerful tool for acoustic wave source engineering. For example, we can achieve lateral scanning without physically separated piezoelectric transducer arrays.

Phase engineering capability

This is an advantage of nano-ultrasonics compared with picosecond ultrasonics. Phase information is crucial in 3-D ultrasonic imaging processing. The ability to design the waveform and phase of the acoustic source with nanometer wavelength also provides a powerful tool for many studies such as elastic property study in the regime of nano-scale and terahertz response.

3-D nano-ultrasonic imaging

To obtain nano-ultrasonic imaging, the acoustic beam size determined by the excitation area of fs pulses also should be on the nanometer scale. This can be done by using nearfield optical techniques. Besides, typical ultrasonic imaging is composed of back-scattered signals. The scattered signal also may provide the information of the crystal quality in a nanometer scale, e.g. defect distributions in the semiconductor samples. To detect the scattered signals, larger amplitude NAW and higher SNR of the optical system are required.

CONCLUSION

We show that quantum nondestructive testing is the new area for ultrasonic nondestructive testing of nanostructures and opaque nanometric multilayers useful for semiconductor industries. The generation of THz nanoultrasonic waves is induced by femtosecond optical pulses. It can produce higher resolution than picoultrasonic which is induced by picosecond optical pulses.Quantum theory is needed for the interpretation of scattered wave signal data within the nanoscale structures.

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