

Multiphysics FEA Simulation for Polymer Nanocomposite Laser Ultrasound Transducer

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Abstract— In this study, the acoustic output of candle soot nanoparticles(CSNP)/PDMS laser ultrasound transducer (LUT) was predicted by a multiscale hierarchical simulation method. Firstly, the carbon/PDMS composites' effective properties were estimated by the nanoscale unit model. Secondly, a LUT model was developed in COMSOL by coupling Wave Optics, Heat Transfer, Structural Mechanics and Acoustics modules, and the acoustic output at the LUT surface was predicted using the properties parameters generated by the model in the first step. Lastly, the near-field wave proportion was calculated theoretically. For CSNP/PDMS LUT, our hierarchical model had high accuracy on both time and frequency domain output.

Keywords—nanocomposite, photoacoustic, laser ultrasound transducer, FEA, multiscale, multiphysics.

I. INTRODUCTION

The laser ultrasound transducer (LUT) has been developed as an emerging technology for high-intensity focused ultrasound (HIFU) [1]–[6]. The LUTs overcome many challenges of the traditional piezo-based transducer with their excellent merits such as high-power density, high frequency, broad bandwidth, and wireless device operation. LUTs employed the optoacoustic effect which converts the laser's energy to acoustic energy [7]–[15]. Firstly, the absorption layer, which usually are composites with high optical absorption embedded particles, absorbs the specific wavelength laser and converts it to thermal energy. The local temperature of the LUT increases dramatically in a very short duration corresponding to the bandwidth of the laser pulse (3

- 10 ns). Secondly, the material volume expands due to the temperature difference. Thermal energy converts to mechanical energy. Lastly, at the surface of the LUT, the acoustic wave was generated. Due to the high energy density and short duration characteristics of the incident laser, the acoustic waves produced by LUT usually have high acoustic pressure and high frequency (10 - 30 MHz) [7], [16]–[18].

As the application areas of LUT have expanded and specialized, there is an emerging need to design a LUT to meet bespoke output characteristics for a wide variety of applications [19]–[22]. For instance, the high axial resolution imaging needs broader -6dB bandwidth; the medical lithotripsy and plaque disruption require high positive pressure; high precision operation ablating malign tumors necessitates both high positive pressure and board -6dB bandwidth to avoid possible damage of surrounding tissue [16], [23]. Carbon/Polydimethylsiloxane (PDMS) is commonly used for optoacoustic nanocomposite due to the high laser absorption coefficient of carbon ($30 \mu\text{m}^{-1}$) and high thermal expansion coefficient of PDMS ($300 \times 10^{-6}/^\circ\text{C}$). It is necessary to understand the relation of the properties of the material with the final acoustic output before researchers design and fabricate the LUTs. Previously, researchers have developed several predicting models based on theoretical calculations or FEA, but there is still a significant discrepancy between the predicted results with the experiments. In this study, a multiphysics and multiscale FEA model was developed to predict the candle soot nanoparticle(CSNP)/PDMS transducer's output.

II. METHODS

A. Effective nanocomposites properties predicting model

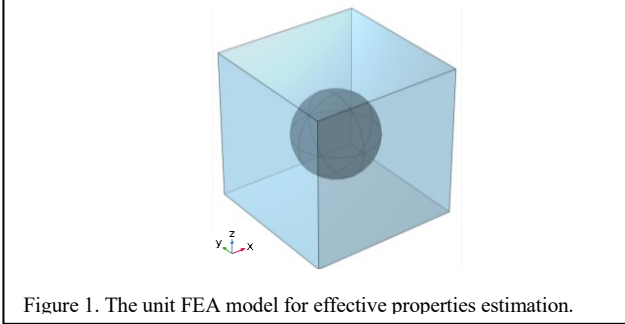


Figure 1. The unit FEA model for effective properties estimation.

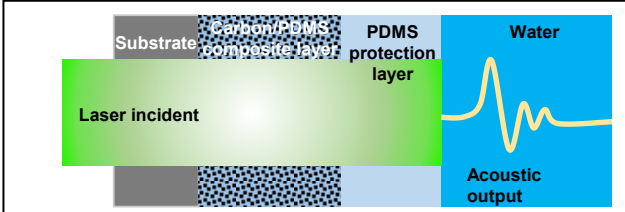


Figure 2. LUT model diagram

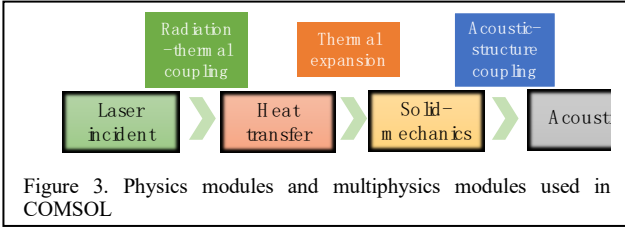


Figure 3. Physics modules and multiphysics modules used in COMSOL

To decrease the computation load of the following FEA LUT model, the effective properties of the absorption layer CSNP/PDMS nanocomposite were estimated by the unit FEA model (Figure. 1) [24]–[28]. Total five physical properties were predicted: absorption coefficient α , Young's modulus E , Poisson's ratio ν , thermal expansion coefficient β and thermal conductivity K . Other two properties, effective density, and heat capacity, were simulated by theoretical equation based on the particles volume fraction.

B. LUT output predicting FEA model

After the effective properties of the nanocomposites were obtained, they are employed in the LUT FEA model. This FEA model was built in COMSOL Multiphysics 5.5. The model includes three layers for LUT and one layer (water) for the media (Figure 2). Four physics modules and three multiphysics modules were used (Figure 3). By using this model, the acoustic output in the time domain at the LUT surface can be achieved with one step.

C. Near field wave propagation calculation

The acoustic wave propagation at the near field was calculated by the theoretical equation:

$$p(\mathbf{r}, t) = -\frac{jk}{2\pi} p_0 e^{-j\omega t} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{e^{ikz}}{z} e^{ik[(x-x_0)^2 + (y-y_0)^2]/(2z)} dx_0 dy_0 \quad (1)$$

where $p(\mathbf{r}, t)$ is the acoustic pressure at a location $\mathbf{r}$ at a time t , k is the wavenumber, p_0 is the acoustic pressure at the

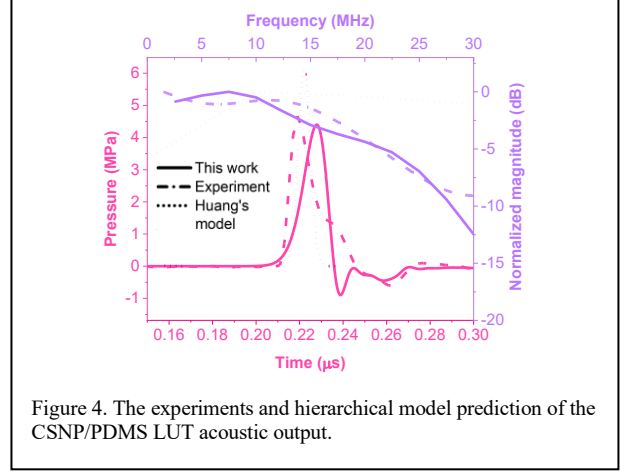


Figure 4. The experiments and hierarchical model prediction of the CSNP/PDMS LUT acoustic output.

transducer surface, ω is the angular frequency of the acoustic wave at the transducer surface.

III. RESULTS AND DISCUSSIONS

The hierarchical predicting method was validated by comparing the experiment results and theoretical calculation (Huang's model) in the literatures [7] and [29], respectively. The CSNP/PDMS in the literature was composed of three layers: glass substrate, CSNP/PDMS layer, PDMS protection layer. All parameters were set as same as the literature. The particle volume fraction is 9 vol%, diameter is 40 nm, the incident laser intensity is 3.57 mJ/cm². Firstly, the CSNP/PDMS nanocomposite effective physical properties were estimated by the unit model. The predicted results were shown in Table 1. Secondly, the effective properties were employed in the LUT FEA model, the acoustic signal at the LUT surface can be obtained. Lastly, the acoustic signal at 4.2 mm was calculated with the LUT surface signal and equation (1). The acoustic output in both the time and frequency domain were shown in Figure 4. All the acoustic output parameters were summarized in Table 2.

For the CSNP/PDMS LUT, the hierarchical model shows excellent accuracy. The predicted peak positive pressure is with 0.2MPa error, peak negative pressure is with 0.29 MPa error, the peak frequency is with 2.51 MHz error, the -6 dB bandwidth is with 1.2 MHz, and the efficiency is with 0.1% error.

TABLE 1. The FEA unit model prediction of the CSNP/PDMS effective properties.

	Glass	Water	PDMS	CB	9% CSNP
β [1/K]	—	—	3.30×10^{-4}	2×10^{-6}	3.02×10^{-4}
C_p [J/(kg×K)]	1000	4200	1460	675	1390
ρ [kg/m ³]	2200	1000	970	1630	1029
K [W/(m×K)]	2	0.65	0.16	150	0.207
α [1/μm]	0	0	0	32	1.31
E [kPa]	72×10^6	—	750	10^7	951
ν	0.17	—	0.49	0.2	0.49

TABLE 2. The Hierarchical model prediction of the CSNP/PDMS LUT acoustic output.

	Peak positive pressure [MPa]	Peak negative pressure [MPa]	Peak frequency [MHz]	-6 dB bandwidth [MHz]	Efficiency
Exp	4.66	0.6	10	22.5	0.45%
Huang	6.1	—	10	65	0.32%
FEA	4.4	0.89	7.49	21.3	0.35%

IV. CONCLUSION

In this research, a novel hierarchical multiscale model predicted the CSNP/PDMS LUT acoustic output with high accuracy. The waveform is very similar to the experiment. The hierarchical predicting model can be used to predict the output of LUT, investigated the optimal design, and analyze the underlying relation between the materials' properties with the LUTs' acoustic output.

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