Ultrafast excitation of water-immersed Carbon Nanotubes: thermophone vs mechanophone effect

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The photoacoustic effect in carbon nanotubes (CNTs) provides a new technique for biomedical diagnostics and treatment in living systems [1, 2] and, in general, a mean for acoustic frequency generation ranging in the THz. However, a thorough understanding of the thermoacoustics properties of a matrix embedded CNT is still lacking. In this context, we theoretically and computationally investigate here the transient photothermal acoustic response of CNTs immersed in water, triggered by an ultrafast laser pulse. Given the time and length scales involved, the system requires a multi-physics, multi-scale approach [3]. First, the laser pulse triggers an impulsive temperature increase of the CNT (sub-ps time scale). Heat is then dissipated to the proximal water portion surrounding the CNT (ns time-scale). The thermal exchange at the CNR/water interface is governed by the thermal boundary resistance [4], which we retrieve from dedicated molecular dynamics (MD) simulations [5]. The CNT and water temperature increase leads to their thermal expansion, finally launching a pressure wave in water.

For similar cases, with water-dispersed metallic nanoparticles excited by nanosecond pulses, only the water's expansion plays an effective role in launching the acoustic wave (thermophone effect) [4, 6]. Here, the contributions of the CNT's and water's expansion are discussed in detail, showing the emergence of a new competitive mechanism, which involves the generation of periodic vibrations or impulsive dilation in the CNT upon pulsed excitation, and the direct mechanical launching of a pressure wave in water (mechanophone effect).

Our simulations follow step-by-step the photothermal-acoustic steps involved, thus combining the optical, heat transfer and thermo-acoustic phenomena. The problem is tackled solving, via Finite Element Methods, the macro-physics equations upon insertion of the microscopic thermal parameters calculated from MD.

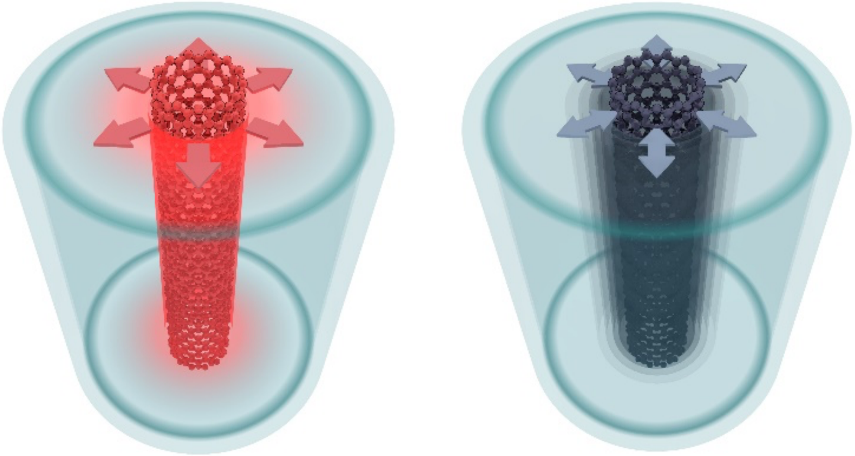

Fig. 1. Schematic representation of the mechanisms for pressure wave generation in water upon nanotube pulsed light excitation. (**Left**) Wave triggered by photothermal dilation of surrounding water, referred to as thermophone. (**Right**) Wave triggered by mechanical expansion of the nanotube, referred to as mecanophone.

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