condition, which has been shown to be important in silicon grain boundaries for example[5]. Such extensions are feasible, however. This work represents an important transformation in the application of *ab initio* techniques to complex systems with unknown structures, and the method is expected to be fruitfully used for many more ceramic grain boundaries and will have many interesting extensions. ❐

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CARBON NANOTUBES

# An explosive thrust for nanotubes

Carbon nanotubes direct chemically produced thermal waves, providing propulsion and thermopower waves that create electrical energy.

Ali E. Aliev and Ray H. Baughman

Carbon nanotubes are efficient guides for electrons and phonons, enabling along their lengths both bullet-like electron flight for micrometre distances and a thermal conductivity that is ten times higher than that of copper[1]. They also guide carbon atom addition at one end of the nanotube during nanotube growth, so that high-perfection nanotubes over 10 cm in length can be produced. The question is, could carbon nanotubes serve as directional guides for other interesting and practically useful chemical reactions?

Writing in *Nature Materials*, Wonjoon Choi and co-workers provide an exciting answer to this question: the authors have demonstrated that carbon multiwalled nanotubes (MWNTs) can guide thermal waves generated by the combustion of cyclotrimethylene trinitramine (TNA; ref. 2), a long-used military explosive. The reaction velocity of TNA coated on the nanotubes is 10,000 times higher than for bulk TNA. Even more interestingly, the authors show that the combustion-produced waves thermally excite electrons and push them along the length of the nanotube. This generates a pulse of thermally excited electrons, called a thermopower wave, which can be harvested as electrical energy.

The team achieved these remarkable results using a well-conceived nanotube architecture that was simple to prepare. An array of vertically aligned MWNTs, sometimes called a nanotube forest, was grown by a conventional chemical vapour deposition method using ethylene precursor gas. TNA was introduced into the forest from solution, with the forest able to accommodate up to 45 times TNA by mass, providing annular shells of TNA as conformal coatings on the MWNTs. A small amount of sodium azide was also added to aid ignition. Choi *et al.* used either laser irradiation or electrical discharge to ignite the propellant at one end of a fibre-shaped chunk of forest; propagation of the thermal wave was then recorded with a microscope-aligned optical-fibre array and a camera operating at 90,000 frames per second. Electrical connections to the nanotube ends and force sensors enabled the measurement of thermopower waves and pressure waves, respectively. The nanotubes guide these waves and it is here that sample preparation comes to the fore; the retention of a high degree of nanotube orientation is essential as arrays with randomly oriented nanotubes did not sustain ignition. Furthermore, reaction-wave pressure measured perpendicularly to the nanotube orientation was much lower than that along the direction of the nanotube.

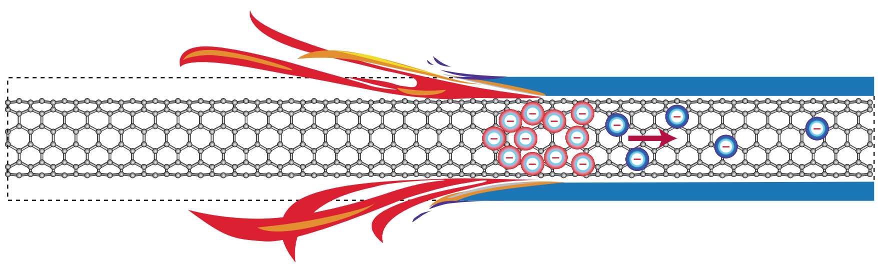

Figure 1 | A chemically driven thermal wave (shown in red) generates thermally excited electrons in a thermopower wave; its propagation to the cold (blue) end of the nanotube can be harvested as electrical energy. Figure courtesy of Ali E. Aliev.

This fascinating ability of the MWNTs to guide a chemically produced thermal wave is a consequence of the exceptionally high thermal conductivity achievable for individual MWNTs, which is at least 3,000 W m$^{-1}$ K$^{-1}$ at room temperature[3]. It is the heat transport along the nanotubes that facilitates the fast combustion of the annular coating of TNA compared with the bulk compound. The authors' note that as it is only those phonons close to the reacting area of the carbon nanotubes that contribute to wave propagation, the reaction wave will undergo giant acceleration if the phonon mean path is commensurate with the length of the reaction zone. They also show that an effective thermal conductivity of ~1,300 W m$^{-1}$ K$^{-1}$ is able to describe the observed reaction velocity along the nanotube orientation direction. As nanotube bundling can decrease thermal conductivity by as much as 10-fold, due in part to quenching thermal vibrations[3–5], the 10,000-fold enhancement of reaction rate depends on realizing a low degree of nanotube bundling.

The specific electrical power generated (7 kW kg$^{-1}$) exceeds that of lithium-ion batteries commercialized for automotive and railway applications (2.6 kW kg$^{-1}$) and vehicle batteries being introduced by Hitachi (4.5 kW kg$^{-1}$; ref. 6). However, the efficiency of converting the chemical



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energy of TNA to electrical energy is no more than 0.3%, which means that the effective electrical-energy storage density is about 2.8 W h $kg^{-1}$, as compared with the 75 W h $kg^{-1}$ for high-discharge-rate lithium-ion batteries[6]. Despite this, the electrical-energy storage density is encouraging, because energy storage density generally decreases with battery size, and no one has yet made a nanometre-diameter lithium-ion battery. Moreover, the authors suggest that control of radiative heat loss could dramatically increase chemical-to-electrical energy conversion efficiency.

Nanotube-guided combustion might also be used for microthrusters — miniature combustion engines sought for purposes such as maintaining relative microsatellite positions within a microsatellite array. The directed pressure wave provides a total impulse (per mass of TNA and MWNT) that is 4–100 times that of other proposed microthrusters[7–9], which is an important figure of merit for determining the weight of microthrusters needed to change the momentum of a microsatellite. Although the efficiency of converting chemical energy to a combination of mechanical and electrical energy is at present low (0.42%), this could probably be increased substantially by using narrower-diameter nanotube arrays having decreased lateral thermal interconnectivity; using a nanotube dopant to optimize thermopower; and by decreasing radiative heat losses. Moreover, energy conversion efficiency might not be especially important for some applications where performance is judged entirely by whether or not a desired electrical or mechanical energy output can be delivered by a device with nanometre-sized diameter, that is for releasing jammed microactuators or microvalves.

As the MWNTs are not destroyed by the 2,860 K temperature that is reached for the thermal waves, it might even be possible to construct a nanotube version of a pulse detonation engine[9] in which perhaps millions of nanotube microthrusters are assembled in parallel, individually fired electronically as desired, and refilled with propellant when needed using a liquid- or gas-phase delivery system.

As is often the case with pioneering fundamental research, the ensuing applications may well turn out to be very different from those initially predicted. Even so, whatever the practical outcomes, the work of Choi *et al.* has certainly taken carbon nanotube research in an intriguing new direction. ❐

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