Gears Based on Carbon Nanotubes

Nanometer size gears could be used in molecular-scale machines.

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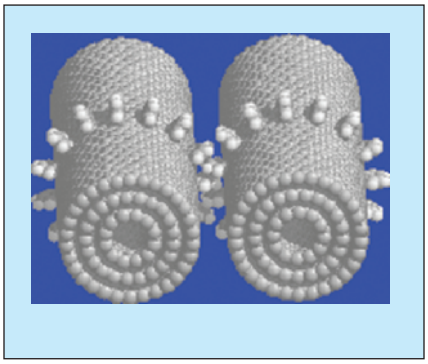
Gears based on carbon nanotubes (see figure) have been proposed as components of an emerging generation of molecular-scale machines and sensors. In comparison with previously proposed nanogears based on diamondoid and fullerene molecules, the nanotube-based gears would have simpler structures and are more likely to be realizable by practical fabrication processes. The impetus for the practical development of carbon-nanotube-based gears arises, in part, from rapid recent progress in the fabrication of carbon nanotubes with prescribed diameters, lengths, chiralities, and numbers of concentric shells.

The shafts of the proposed gears would be made from multiwalled carbon nanotubes. The gear teeth would be rigid molecules (typically, benzyne molecules), bonded to the nanotube shafts at atomically precise positions. For fabrication, it may be possible to position the molecular teeth by use of scanning tunneling microscopy (STM) or other related techniques. The capability to position individual organic molecules at room temperature by use of an STM tip has already been demonstrated. Routes to the chemical synthesis of carbon-nanotube-based gears are also under investigation.



Two Molecular-Scale Gears are shown meshing in this computer-simulation image. The gears would include multiwalled carbon-nanotube shafts, to which gear teeth in the form of benzyne molecules would be bonded.

Chemical and physical aspects of the synthesis of molecular scale gears based on carbon nanotubes and related molecules, and dynamical properties of nanotube-based gears, have been investigated by computational simulations using established methods of quantum chemistry and molecular dynamics. Several particularly interesting and useful conclusions have been drawn from the dynamical simulations performed thus far: The forces acting on the gears would be more sensitive to local molecular motions than to gross mechanical motions of the overall gears. Although no breakage of teeth or of chemical bonds is expected at temperatures up to at least 3,000 K, the gears would not work well at temperatures above a critical range from about 600 to about 1,000 K. Gear temperature could probably be controlled by use of coolant gases. For a given application, the gears would work well at temperatures below the critical range, provided that the rotational energy was less than the energy required to tilt the teeth through an angle of 20°. The predominant mechanism of gear failure would be slippage caused by tilting of teeth. Gears would resume functioning if the slipping gears were decelerated sufficiently.

This work was done by Richard Jaffe of **Ames Research Center***; Jie Han and Al Globus of MRJ, Inc.; and Glenn Deardorff of Sterling Software. Further information is contained in a TSP (see page 1).*

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