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Machine phase fullerene nanotechnology

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Abstract. Recent advances in fullerene science and technology suggest that it may be possible, in the distant future, to design and build atomically precise programmable machines composed largely of functionalized fullerenes. Large numbers of such machines with appropriate interconnections could conceivably create a material able to react to the environment and repair itself. This paper reviews some of the experimental and theoretical work relating to these materials, sometimes called machine phase, including the fullerene gears and high-density memory recently designed and simulated in our laboratory.

1. Introduction

Advanced materials are routinely used in the construction of aerospace vehicles. Despite many advances, transportation to space still costs about $10 000 per lb. Drexler (1992) proposed a nanotechnology based on diamond and investigated its potential properties. These studies and others suggest enormous potential for the role of diamonoid nanotechnology in aerospace systems (McKendree 1995). In particular, McKendree (1995) estimated $150–400 per lb transportation cost to orbit assuming naive use of diamonoid molecular nanotechnology to improve existing launch vehicle designs.

Unfortunately, methods to realize diamonoid nanotechnology are at best highly speculative. Recent computational efforts at NASA Ames Research Center (Globus *et al* 1996) and computation and experiment elsewhere suggest that a nanotechnology based on machine phase functionalized fullerenes may be synthetically *relatively* accessible and possess great potential for aerospace applications. This nanotechnology might use carbon nanotubes and related components as the building blocks of molecular machines. Carbon nanotubes (Iijima 1991) are rolled up sheets of hexagonal graphite that form single- or multiwalled tubes. Typically, these tubes have caps with six pentagons each that add curvature to form closed molecules.

Machine phase materials are (often hypothetical) materials consisting entirely or in large part of microscopic machines. In a sense, most living tissue fits this definition since it is composed in large part of protein ‘machines’. As a result, for example, our skin is able to sense its environment, react to it, change shape as we grow, and repair itself. Thus, although skin is not particularly strong, it routinely lasts 80 or more years in an often hostile environment.

A viable general purpose machine phase technology requires, at a minimum, mechanical motion, cooling, power, support structures, control, a variety of physical components, a system architecture, and some approach to manufacture. Except for the system architecture and manufacturing, there is some experimental or simulation basis for all of these areas. The rest of this paper investigates each area in turn; but first we briefly review the known and computed properties of carbon nanotubes relevant to machine design. Note that the references in this paper are not meant to be a complete review of fullerene nanotubes.

Carbon nanotubes are extremely strong and flexible. Treacy *et al* (1996) observed an exceptionally high Young’s modulus for individual multiwalled carbon nanotubes (0.40–3.7 TPa). Yacobson *et al* (1996) calculated a Young’s modulus of 5.5 TPa for single-walled carbon nanotubes. Apparently, when calculating Young’s modulus some authors use the full disk as the cross sectional area and others use a ring with an open center. This, of course, results in different values. Care should be taken when reading the literature (Yacobson *et al* (1996) uses a hollow core). In any case, these strength studies should not be considered definitive.

Yacobson *et al* (1996) made a theoretical study placing single-walled carbon nanotubes in axial compression. They found that the tubes compressed continuously with occasional singularities corresponding to shape changes as buckling adds waves to the system. Srivastava and Barnard (1997) found that axially compressed multiwalled nanotubes behave differently than single-walled nanotubes because of the long-range tube–tube interactions which are not present in single-walled nanotubes.

Iijima *et al* (1996) reported on experiments and simulations of bending carbon nanotubes. They noticed

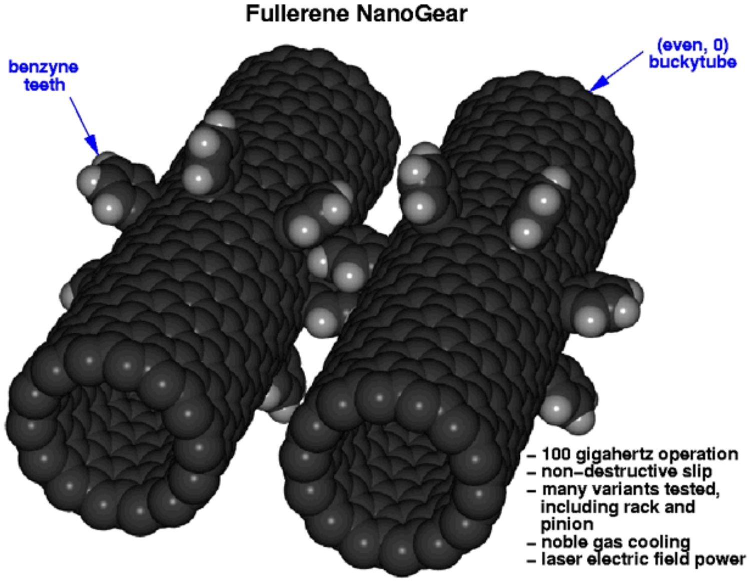

Figure 1. Fullerene gears made from carbon nanotubes and benzyne teeth. Gray spheres are carbon atoms, white spheres are hydrogen.

that nanotubes bent to a 30° angle develop kinks but the hexagonal bond pattern remains intact up to about 110°. This suggests that even when tubes are substantially deformed, they can return to their original state.

Satishkumar *et al* (1996), Ugarte *et al* (1996) and others have opened the ends of nanotubes, filled them with various metal compounds, and closed the ends.

Lee *et al* (1997) and Rao *et al* (1997) reported in companion papers that single walled carbon nanotubes doped with bromine or potassium exhibit increased conductivity at 300 K by a factor of 30, suggesting that doped nanotubes represent a new family of synthetic metals. Raman scattering measurements suggest that the doping increases carrier concentration.

Carbon nanotubes with different diameter and helicity are commonly described by two numbers, for example, (10,10), (9,0), etc. To understand this notation, 'start with a point on a graphitic sheet, take an integral number of steps along one crystallographic axis, followed by another (and typically different) integral number of steps along the second crystallographic axis, reaching an endpoint. The straight line connecting the start point and the endpoint is then defined as the circumference' of the carbon nanotube—Ralph Merkle.

For an excellent overview of fullerene science including carbon nanotubes see Dresselhaus *et al* (1995). For a more recent review of carbon nanotubes see Ebbesen (1997).

2. Mechanical motion

Tuzun *et al* (1995a) used molecular dynamics to investigate the properties of bearings consisting of an inner and an outer carbon nanotube. They found that performance was dominated by vibrational effects but smooth rotation could be achieved with careful choices of temperature, velocity and size.

To begin the investigation of fullerene nanotechnology at Ames, we used molecular dynamics to study the properties of carbon nanotube based gears and gear/shaft configurations Han *et al* (1997b). Experiments on C60 Hoke *et al* (1992) have shown that C60 combines with benzyne in a 2 + 2 cycloaddition reaction under mild conditions. Jaffe and Han (1997a) matched these results with quantum calculations, matched the 2+4 cycloaddition reaction of benzyne and naphthalene Hoffmann (1967), and went on to show that benzyne attached to the side of a carbon nanotube with 2 + 2 and 2 + 4 cycloadditions is stable. The relative stability of each product varies with the diameter and helical winding of the tube as well as the orientation of the benzyne adduct. Our fullerene gears are formed (in software) by adding these relatively stiff benzyne fragments around the tube to make teeth (see figure 1).

Han *et al* (1997b) used Brenner's potential Brenner (1990) to computationally demonstrate that molecular gears fashioned from (14,0) single-walled carbon nanotubes with benzyne teeth spaced every two rings around the tube's circumference should operate well at 50–100 GHz. Brenner's potential is a classical, reactive hydrocarbon potential parameterized to fit diamond, graphite, and small hydrocarbon molecules. A software thermostat kept the temperature at 200 or 300 K (depending on the simulation run). Software springs were attached to atoms at the end of each tube to simulate a support system, and atoms near the ends of one (powered) tube were given an angular velocity increment each time step to simulate a motor. At rotation rates below about 100 GHz, rotation of the powered gear induces rotation of the other (driven) gear. At rotation rates above 100 GHz the teeth slipped past each other. However, bonds were not broken (Brenner's potential is reactive) so that when rotation rates were reduced the gears began functioning again.

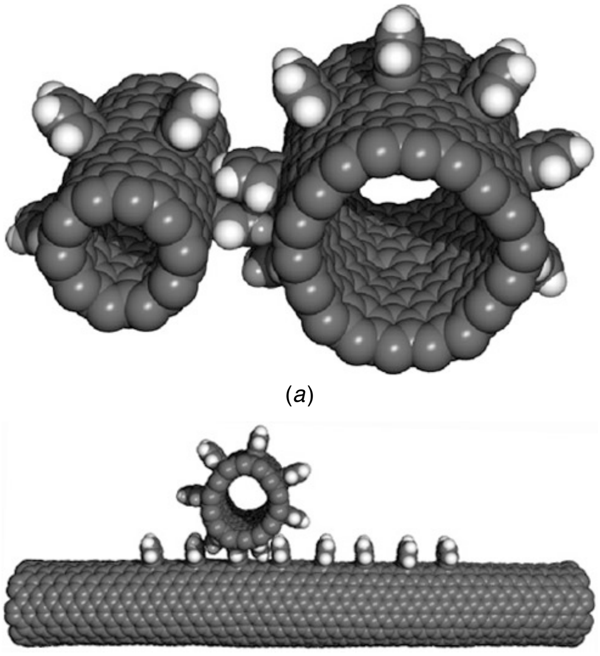

Figure 2. (*a*) Fullerene gears of different sizes. Computational experiments suggest that applying power to the large gear works much better than applying power to the small gear. (*b*) Fullerene rack and pinion system. Teeth are spaced two rings apart on the gear but three rings apart on the shaft. This is required since on the gear the teeth diverge whereas on the shaft they do not. In each case sufficient space must be available to mesh with teeth on the other component.

Han *et al* (1997b) also investigated systems involving large (18,0) and small (10,0) gears. When power was applied to the large gear, the system worked well. However, when power was applied to the smaller gear, a very complex motion resulted and the larger gear did not rotate substantially, perhaps because the larger gear had too much inertia (see figure 2(*a*)).

Han *et al* (1997b) also investigated a rack and pinion system. Here a gear meshes its teeth with teeth spaced every three rings along the long axis of a (9,9) tube. Spacing every three rings, rather than every other ring as works on the gears, is necessary for the opening between teeth to be large enough (the teeth are parallel rather than divergent). The rack and pinion system was able to convert rotation of the gear into linear motion of the (9,9) tube and linear motion of the (9,9) tube into rotation of the gear (see figure 2(*b*)).

While the gears appear to work well, at least in simulations, synthesizing them presents problems. First, the gear teeth must be added at precise positions but there is no particular reason for a reaction to prefer one site over another. Worse, fullerene nanotubes are much like the surface of a graphite sheet, which is not very reactive. The curvature of the tubes gives the primarily SP2 carbon atoms some SP3 character—particularly for small radius tubes, but apparently not enough to easily functionalize them. SP3 character for a carbon atom with only three neighbors creates a reactive radical site. However, computation and experiment have shown that bending (Ruoff and Lorentz 1995) or compressing (Yacobson *et al* 1996) tubes causes buckling. Some of the atoms, where the tube buckles, must have substantial SP3 character. Therefore, we predict that bending carbon nanotubes sufficiently to cause buckling will allow fairly precise functionalization of the nanotubes. This may be a route to adding gear teeth to nanotubes.

Robertson *et al* designed a gear system based on fullerenes and described it on the World Wide Web. Cagin *et al* (1997) investigated a diamonoid planetary gear.

Our group has conceptually designed a number of other components, including hinges, springs, universal joints and other systems. However, we have not yet investigated these systems in detail.

3. Cooling

Han *et al* (1997a) investigated cooling fullerene gears in an inert atmosphere. A neon or helium atmosphere was added to the (14,0) gear system. The software thermostat was removed from the gears and applied to the atmosphere. In initial simulations, the gears no longer turned so the software motor was modified. Instead of adding angular momentum to the end atoms of the powered gear, their position was updated each simulation step and this position was not allowed to change in response to interatomic forces. This simulates a more powerful motor. The gears turned and the temperature eventually stabilized, i.e. the atmosphere was able to control the temperature of the gears.

4. Power

Tuzun *et al* (1995b) simulated using a laser to turn carbon nanotubes. In these simulations, unit positive and negative charges were added to two carbon atoms on opposite sides of a nanotube, and an electric field was added simulating one or more lasers. The tubes turned but the direction alternated, undesirable behavior for a motor. Srivastava (1997a) simulated using alternating electric fields generated by a single simulated laser to power Han's fullerene gears. In these simulations, the software motor was removed, unit positive and negative charges were added to two carbon atoms on opposite sides of the powered nanotube, and a 140 GHz alternating electric field was added simulating a laser. The proper frequency was found using a linearized approximation of a phenomenological equation describing the system. The laser-powered gear system rotates consistently in one direction, although we are unable to predict whether rotation will be clockwise or anticlockwise. Interestingly, Srivastava (1997b) discovered that a pulsed laser worked better than a continuous laser. When the laser was off, the gears slowed down and cooled but rapidly sped up when the laser came on again. Since the initial start-up of the gears must overcome static friction, a great deal of heat was generated. On the other hand, adding power to moving gears must only overcome dynamic friction which generates less heat. The pulsed laser resulted in a cooler system.

Tsai and Tahmasebi (1993) and Tahmasebi and Tsai (1995) proposed a six-degree-of-freedom (DOF)

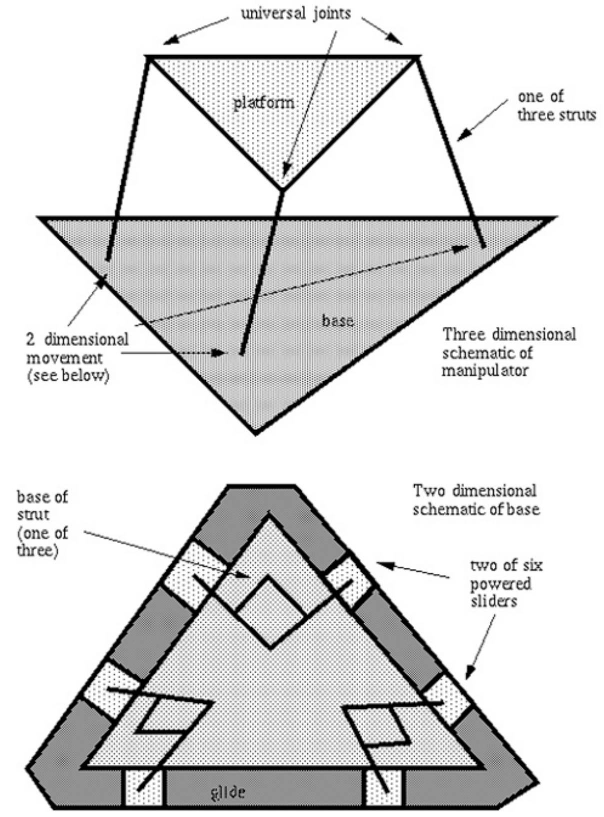

Figure 3. Six DOF manipulator with relatively few components. Figure is redrawn with permission from Tsai and Tahmasebi (1993).

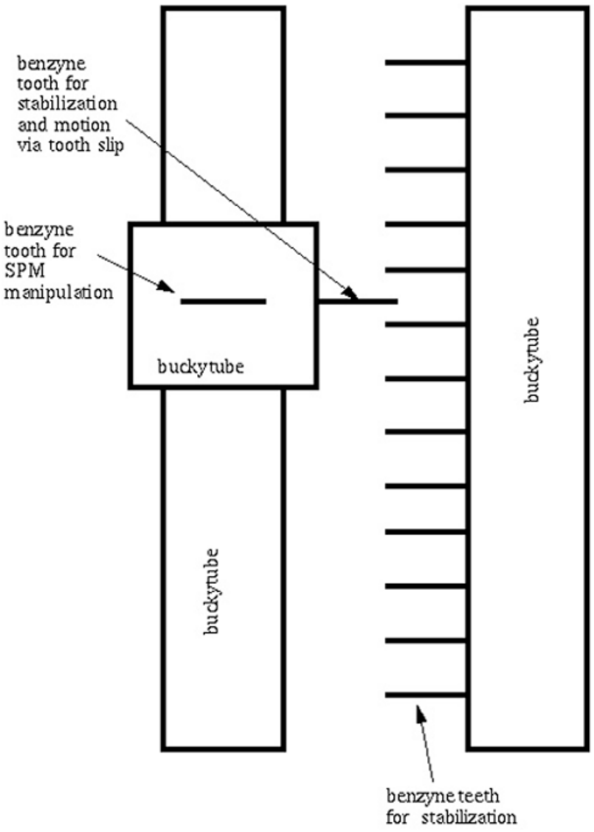

Figure 4. Schematic diagram of fullerence system for powered linear motion using SPM for power and control.

minimanipulator of remarkably simple design (see figure 3). In particular, this manipulator requires only one-dimensional linear motion for power and control. This power must be applied to components mounted on a planar base on which the rest of the manipulator is mounted. If the powered components have a small tab (for example, a benzyne ring attached to a carbon nanotube) protruding from the base of the manipulator on the opposite side from the rest of the unit, then a single-carbon nanotube-tipped scanning probe microscope (SPM) (Dai *et al* 1996) could be used to power and control the system. For this to work, the powered components would need to stay put once positioned. This could be accomplished by meshing another benzyne ring on the powered tube with a series of benzyne teeth on a support structure. The teeth can be made to slip when pushed hard enough, but will hold the powered tube in position while the SPM is used to control other powered elements. Tooth slip can be enhanced by minimally overlapping the meshed teeth (see figure 4). Such a system, although very slow and as yet poorly analyzed, would use only existing SPM technology for both power and control.

5. Support structures

Theory (Dunlap 1992, 1994a, b) and experiment (Zhang and Zhang 1995) suggest that fullerene tubes may be joined at 30° angles to create complex structures including helices. Theoretical models of three-way-joined tubes have appeared in the literature (Colbert and Smalley 1995), but there is no experimental evidence of such structures. Such evidence would be of great value in the design of support structures.

Multiwalled carbon nanotubes have been observed with broken outer walls (Sattler 1996). This suggests that an open-ended nanotube can exist surrounding a longer nanotube. This would allow components to be stabilized in all directions except along the tube axis. Strategically placed benzyne rings added to the inner tube could be used to constrain motion of the outer tube along the tube axis.

6. Control

First, we remind the reader of the discussion in the power section suggesting that control of a primitive six DOF manipulator appears possible using existing SPM technology. More complex control systems usually require computers at their heart. While no one has built a fullerene computer, computational studies suggest that a number of promising computer components could be built, at least in theory. Thus, we will investigate fullerene computers first.

Joachim and Gimzewski (1997) has created an electromechanical switch using a single C_{60} molecule held between an STM tip and a conducting substrate. Current passed through C_{60} by the STM changes substantially and reversably when the STM tip deforms the molecule. The speed of the switch is a function of the speed of mechanical deformation, limited only by the vibrational frequency of C_{60}—approximately 10 THz.

Theory (Dresselhaus *et al* 1995, pp 802–14) suggests that single walled carbon nanotubes can have metallic or semiconductor properties depending on the helical winding of the tube. (Dresselhaus *et al* 1995, pp 903–4) proposed a number of computer device components based on this property. Dunlap (1992, 1994a) has supplied a theoretical foundation for one way to join nanotubes with different electronic properties together using pentagon and heptagon defects on opposite sides of a nanotube to change the helical winding. Recent calculations (Chico *et al* 1996) suggest that tubes with different helical windings joined by a pentagon–heptagon pair can have different electrical properties at different positions. Experiment has shown that single-walled carbon nanotubes are quantum wires (Bockrath *et al* 1997). Langer *et al* (1996) demonstrated that the conductance of multiwalled nanotubes can be increased by applying a magnetic field perpendicular to the tube axis; which may have applications in data storage. This effect has been demonstrated at temperatures below 4.2 K. Combining these components, and others that may be found, into a computer architecture is a significant challenge for the future.

Bauschlicher *et al* (1997) computationally studied storing data in a pattern of fluorine and hydrogen atoms on the (111) diamond surface using a one-dimensional model (see figure 5). If (presumably write-once) data could be stored this way, 10^{15} bytes/cm^2 is theoretically possible. Bauschlicher *et al* (1997) compared the interaction of different probe molecules with a one-dimensional model of the diamond surface. They found some molecules that had interaction energies with H and F that were sufficiently different that the difference in force should be detectable by an SPM. These studies were extended to include a two-dimensional model of the diamond surface and two other systems besides F/H (Bauschlicher and Rossi 1997). Other surfaces, such as Si, and other probes, such as those including transitional metal atoms, have also been investigated (Bauschlicher and Rossi 1998).

Among the better probes was C_5H_5N (pyridine). We have shown that pyridine attached to C_{60} in the orientation necessary for sensing the difference between hydrogen and fluorine should be stable. Half of C_{60} can form the end cap of a (9,0) or (5,5) carbon nanotube and carbon nanotubes have been attached to an SPM tip (Dai *et al* 1996). Thus, it should be possible using today's most advanced laboratory techniques to build a system to read the diamond memory surface.

Avouris *et al* (1996) has shown that individual hydrogen atoms can be removed from a silicon surface. If this could be accomplished on diamond in a gas that could donate fluorine to the diamond surface, the memory system could be built. Thummel and Bauschlicher (1996) computationally investigated methods for adding an F at the radical sites where a H atom had been removed from a diamond surface.

Mitre maintains an excellent World Wide Web page with links to their survey papers on nanoelectronics, which includes brief discussions of fullerene-based electronic components.

7. Physical components

Fullerenes such as C_{60} have been functionalized by a wide variety of molecular fragments (Taylor and Walton 1993). Satishkumar *et al* (1996) has functionalized nanotubes with an acid solution.

Carbon nanotubes have been observed with a wide variety of ends, including a variety of cap shapes (Ajayan *et al* 1993), and tubes that first reduced diameter for some distance before ending (Iijima *et al* 1992).

Iijima (1993) and Sattler (1996) observed cone-like fullerene objects. Liu *et al* (1997) observed fullerene tori. Endo *et al* (1995) observed spindle-shaped objects. Ebbesen and Takada (1995) observed multiwalled nanotubes whose diameter gradually increased, presumably from the presence of many pentagon–heptagon defects.

Amelinckx *et al* (1994) observed multiwalled fullerene helices, Zhong-can *et al* (1997) explained their ratio of pitch to radius on energetic grounds. Dunlap (1994b) provided a theoretical basis for single-walled helices with pentagon and heptagon defects. Ihara and Hou (1995) developed several theoretical ways to construct fullerene torii and helices and computationally determined that the spring constant for helical C_{360} is 4.09 meV nm^{-1} and for helical C_{540} is 0.16 meV nm^{-1}. We have derived a generized topological construction method to join nanotubes into bends with angles of 0–30° by introducing pentagon–heptagon pairs at different separations.

It therefore seems reasonable that a variety of shapes could be designed and synthesized. When we designed the gears in Han *et al* (1997b), very little searching of the design space was necessary. Actually, the second design attempted was eventually published. We were either very lucky, or the design space is well populated with potentially useful devices.

8. System architecture

We have an extremely preliminary concept called the replicating swarm. The swarm consists of roughly spherical nodes capable of attaching to five edges (for a tetrahedral geometry with one free edge per node) and rotating each of them in pitch and yaw (see figure 6). The linear edges are capable of changing length, rotating around their long axis, and attaching/detaching to/from nodes. Both components have internal computers, sense force, and can pass data and power to each other. The swarm grows by assembling synthetically generated fullerene components into nodes and edges. When a swarm is large enough, it divides into two by letting go of the appropriate edge/node connections.

Besides the obvious and severe difficulties of building the components and physically connecting them, the software problems in planning and controlling the swarm's actions are daunting. However, these problems could be addressed in simulators with simulated swarm components. Such a simulator could also be used for research into the range of capabilities swarm components should use. One

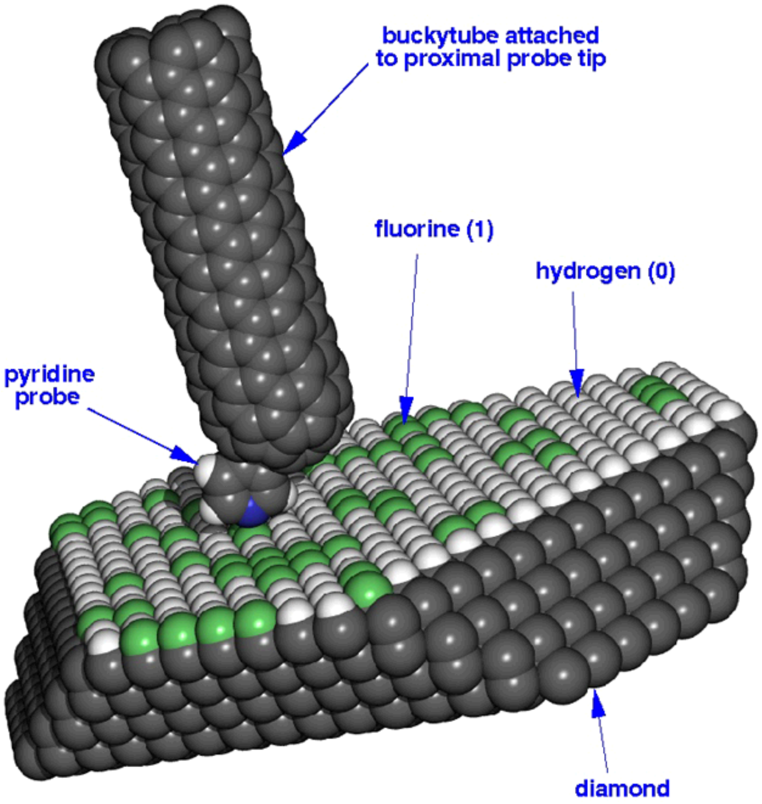

Figure 5. Functionalized carbon nanotube sensing flouring versus hydrogen on a diamond surface. The blue sphere is nitrogen, green spheres are flourine.

author suspects that genetic programming may be a fruitful approach to the software control problem.

9. Manufacture

Multiwalled carbon nanotubes were discovered in 1991 by Iijima (1991). Bethune *et al* (1993) and Iijima and Ichihashi (1993) reported observing single-walled carbon nanotubes in the same issue of *Nature*. Ebbesen and Ajayan (1992) and Thess *et al* (1996) demonstrated high-yield synthesis of multiwalled and single-walled nanotubes respectively. As mentioned above, Satishkumar *et al* (1996) has functionalized nanotubes with an acid solution. Given the history of C_{60}, the next few years should witness an explosion of functionalized nanotube syntheses; some, perhaps, with properties amenable to machine phase materials.

Li *et al* (1996) developed a method to grow 0.05 mm multiwalled nanotubes in aligned arrays on a silica surface. The spacing is controlled by the spacing of iron nanoparticles embedded in the mesoporous silica. Most of the iron particles are believed to be near the bottom of holes in the silica. These cavities apparently orient the nanotubes to be approximately normal to the silica surface. Growing nanotubes in predictable, regular arrays should make modification to useful products easier.

Conceptually, we envisage a reasonably mature fullerene nanotechnology manufacturing system in which small molecular components are generated synthetically in bulk and fed to one of the swarms described above. The swarm assembles swarm edges and nodes from the molecular components thereby growing and eventually dividing. Of course, one needs an initial swarm to begin this process.

Dai *et al* (1996) demonstrated that individual carbon nanotubes can be attached to a scanning probe microscope (SPM) tip. SPMs can manipulate their tips with subangstrom accuracy. The end of carbon nanotubes should have a chemistry similar to C_{60}. C_{60} can be functionalized with a wide variety of molecular fragments (Taylor and Walton 1993). Thus, with some further development it should be possible to synthesize a wide variety of molecular structures using mechanical control to guide reactions of individual molecules. This should allow construction of extremely small quantities of many otherwise inaccessible atomically precise products; for example, swarm components.

10. Conclusions

We see that there is some evidence that fullerene-based machines and, conceivably, machine phase materials based on them may be possible. Combined with the apparently remarkable mechanical and electrical properties of carbon nanotubes, there is some reason to believe that a focused effort to develop fullerene nanotechnology could yield

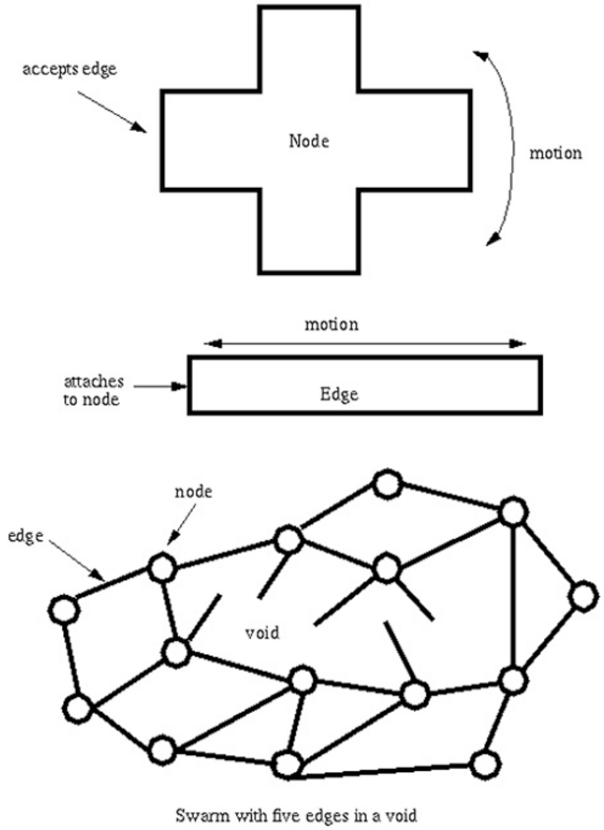

Figure 6. Schematic diagram of a two-dimensional swarm with node and edge details. Edges in the void are available to manipulate objects.

materials with remarkable properties. Materials with electrical properties that could revolutionize circuit design and increased strength-of-materials leading to, among other things, opening the space frontier by radically lowering the cost of launch to orbit. We hope that others will join us in a long range, high risk, potentially enormous payoff effort to develop machine phase fullerene materials.

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