Chapter 27
Mathematical Background for Nanotechnology:
A Survey

Raynetta Prevo-Williams
Alabama State University, USA

Fred Roush
Alabama State University, USA

ABSTRACT

The authors present what they feel to be the most important mathematical background for nanotechnology, with some discussion of this material. They include quantum mechanics of photons and electrons presented historically and with a view to applications in chemistry, computational methods of quantum mechanics, molecular dynamics including Brownian motion, crystal and quasi-crystal structure, automaton theory, fluid dynamics, and quantum computation.

INTRODUCTION

Nanotechnology is one of the most active and promising areas of twenty-first century technology. It has made many contributions to improvement of existing technologies as well as developed new ones.

Nanotechnology has been investigated as a means to treat cancer. Nanoparticles of gold are coated with antibodies that attach to that particular cancer and with a compound like hydrogen peroxide that can kill cells. They are released into the bloodstream and when they pass the tumor, they should attach and kill the cancerous cells. A student won an Intel science award for using carbon nanotubes to detect cancer. Antibodies are placed in the tubes and they swell if the antigen is present. Bergin, et al, 2008 is related to this work.

It has been discovered that some ancient technology involved nanoparticles: the making of Damascus swords uses nanoparticles of steel and the making of stained glass windows involves nanoparticles used to color the glass. It has also been discovered that nanoparticles are important in nature: volcanic ash, sea spray, and smoke have nanoparticles.

Most recently scanning tunneling microscopes have been developed and can see individual atoms and also manipulate them. For instance, Rice University scientists have built a car which is a single molecule. See nanocar Rice University or Wikipedia, nanocar or Shirai, et al, 2005; it does

DOI: 10.4018/978-1-4666-6363-3.ch027

role on a gold surface. Electrons from a scanning tunneling microscope give it some power but it can't steer yet.

Cited in Discover Magazine, Dec. 2012: a computer element storing one bit of information has been developed using only 12 iron atoms; a transistor has been developed using a phosphorus atom embedded in hydrogen-coated silicon (Fuechsle, et al, 2012); a quantum computer with little decoherence has been built. May 2013 reports were published about construction of a laser the size of a virus (Odom, et al, 2012). Related to this work is Loth, et al, 2012.

Also in Science News Letter Dec. 13, 2012: carbon nanotubes coated with paraffin make artificial muscles (Foroughi, 2012), and at Stanford, Anatoly Yakovlev and Daniel Pivonko (Pivonko and Yakovlev, 2012) constructed a several millimeter sized sub to go through the body using an external magnetic field as power. The week of May 8, 2013 reports that a DNA transistor has been constructed, which could be the start of a type of DNA computers and control mechanisms. See Endy, et al, 2013 for related work.

The 2012 winners of the Feynman Prize in nanotechnology have used scanning probe microscopy to give images of molecular orbitals and to precisely make and break chemical bonds. Whereas, the 2006 winners of the Feynman prize developed tiles of crystalline DNA, and showed that algorithmic self-assembly can work. Previous theory relating to this was in Winfree, et all,1998.

Nanotechnology-enhanced paints are on the market. They are nontoxic yet can destroy bacteria and inhibit growth of fungi. It has been shown that incorporating nanoparticles in fabrics can make them stain and water-resistant, kill bacteria, provide superior insulation, and cause dirt to rinse off (Siegfried, 2009).

A more practical use of nanotechnology is to produce tennis balls and tennis rackets that last longer and have other desirable properties, and car wax with nanotechnology can fill in cracks better (Soutter, 2009; Shovlin and Taddie, 2010). There are also products used to keep eyewear cleaner, dryer, and more long-lasting. It can also be used to make photographs have sharper, more realistic images. See also Wang, 2013.

Although mathematics is not at the center of these developments, we feel that it is relevant and important for them. The basis of small-scale study of fluids and gases, and particles in them, is a combination of fluid mechanics and statistical mechanics. Small-scale study of solids involves consideration of crystal structure. At a still smaller scale the fundamental laws for nanotechnology are those of quantum mechanics, and many of the more remarkable properties of nanomaterials, such as nanoparticles of gold, cannot be explained without quantum mechanics. On the other hand, at present the still more complex portions of physics, quantum field theory and the theory of nuclear forces, are not very important for most nanotechnology. There is much interest in constructing nanomechanisms which can be controlled to a considerable extent, and even exhibit machine intelligence. For these kinds of mechanisms, automaton theory can offer guiding principles. It is not yet established whether quantum computers can really be useful but they have fascinating possibilities. In the next section our discussion of quantum theory, is a brief historical development. Since this material is so new, there are not many books on it as a whole, thus our major source has been the Internet. Since the focus of this chapter is on background, a discussion of issues and problems has been incorporated.

BACKGROUND: FLUID MECHANICS

Fluids can be gases, typically thought of as compressible and satisfying some principle like Boyle's law, or liquids, typically thought of as incompressible and preserving volume in their flow. They can also be viscous, or thick, or they can be freely flowing, as water does approximately.