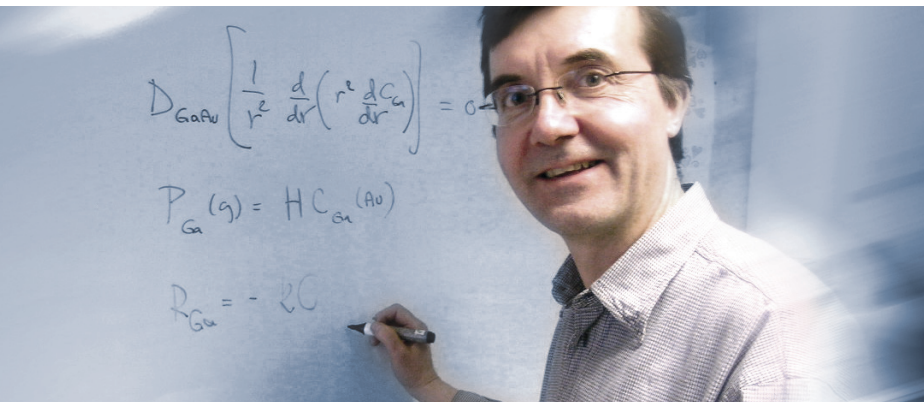


SPINNING

OF THE TINIEST SIZE IMAGINABLE

THREADS



Prof. Stig Stenström from the Chemical Engineering Department at Lund University created a COMSOL Multiphysics model of nanowire growth to help researchers understand and better exploit the underlying phenomena.

Pick up a human hair, and then realize that a nanowire can be a thousand times thinner. Made of materials such as semiconductors, polymers, and carbon, these incredibly thin threads can have diameters < 10 nm, just tens of atoms across. Early laboratory findings indicate that these ultra-fine wires will open up a variety of remarkable applications. But until we learn how to manufacture them efficiently, these commercial uses will remain only dreams. Researchers thought they had a good grasp on how nanowires grow, but recent mathematical models along with laboratory observations have uncovered evidence that a completely different growth mechanism might be at work.

Because of their unique and unusual properties, nanowires offer an amazing range of potential applications. They could serve as wound dressings or drug-delivery systems; allow the design of solar sails and mirrors for outer space; develop innovative agricultural pesticides; act as structural elements in artificial organs; and strengthen reinforced compos-

The process of manufacturing nanowires—the smallest possible threads—is not wholly understood. Sophisticated modeling is helping researchers better understand this revolutionary process and prepare it for commercialization.

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ites. A bed of “nanograss” could result in low-friction surfaces on which substances simply glide off. One near-term use is to implement the interconnects needed to wire together the next generation of integrated circuits, which are shrinking so small that conventional packaging techniques are large and cumbersome in comparison; they can themselves even implement digital logic gates. In the future we can expect to see untold numbers of products and devices that exploit these tiny structures.

A totally new way of looking at the process

In the semiconductor area, the most common method of creating a nanowire is known as the vapor-liquid-solid (VLS) growth mechanism (Figure 1). The process supplies the reactants in a vapor phase. They react with a liquid metallic seed particle placed on a substrate, and a nanowire grows perpendicular to the substrate. The VLS mechanism implies that the solid wire forms through precipitation on a droplet of metal that acts as the seed. The driving force for

crystallization is supersaturation within the droplet, which is established by catalytic absorption of the gaseous reactants from the surroundings.

The manufacturing process (Figure 1) starts with a single crystalline GaAs substrate. The next step is to precisely deposit gold nanoparticles on the substrate, which then goes into a reaction chamber. The chamber is evacuated and heats up to 540 °C. The process then introduces reactants into the chamber as molecular beams of gallium and arsenic. Under the right conditions, GaAs forms under the gold particle but not anywhere else on the surface. The resulting nanowire can grow to be as long as 0.5 to 10 μm. Researchers are concentrating on the parameters that control nanowire growth so it forms semiconductor compounds with desirable properties. Among the factors to control are pressure in the reaction chamber, the concentrations of arsenic and gallium, and the diameter of the gold seed.

In some cases, however, this explanation of nanowire growth leaves many unexplained phenomena and inconsistencies. Scientists clearly need a better understanding of the mechanisms governing semiconductor nanowire growth to enable the development of this promising field. One group of researchers investigating this area comes from the Nanometer Structure Consortium at the Lund Institute of Technology (Lund, Sweden). Members of the physics, materials chemistry, and chemical engineering departments believe that the actual growth mechanism in some cases involves solid-phase diffusion rather than the VLS mechanism. To study this concept, they perform laboratory experiments and compare the results to finite-element calculations of the mass transport and expected growth rates using COMSOL Multiphysics. In this way they hope to clarify the alloying situation and the aggregation state of the seed particle, which is a key to a more complete understanding of the nanowire growth mechanism.

A close look at the seed

To better understand what happens in the reaction zone, the consortium enlisted the assistance of Prof. Stig Stenström from the Chemical Engineering Department, who created a model of growth including transport and the formation of the GaAs compound. This single-physics problem in 3D sets up the material balance and calculates the mass-transfer rate using the Convection and Diffusion application mode. This mode's PDE templates provide the necessary description of the mass-transport equation, but Prof. Stenström had to add a custom equation that accounts for the reaction rate at the substrate layer. Further, he modeled the gold droplet to consist of a

short cylinder topped with a half-sphere.

He also had to apply special techniques when creating the model geometry. The gold spray results in a semispherical droplet on the substrate, and the diffusion at the outer edge is far faster than the diffusion in the middle of the droplet. The resulting model has 4600 nodes and 23,000 elements and solves in just two or three minutes.

Figure 2a shows a typical output plot from the model showing the gallium concentration in the seed particle and the nanowire's growth rate. By integrating the flux of gallium it is possible to calculate the growth rate of GaAs for different process conditions.

One thing that this model showed the researchers was that the previous generally accepted theory of nanowire growth, the vapor-liquid-solid (VLS) mechanism, should be replaced by a vapor-solid-solid (VSS) mechanism.

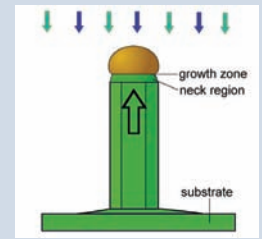


FIGURE 1: To grow a nanowire, the process starts with a seed particle on a substrate. The nanowire's constituents, arsenic and gallium, are supplied as molecular beams, here shown coming from the top. Progressive crystal growth takes place in the zone just underneath the seed particle.

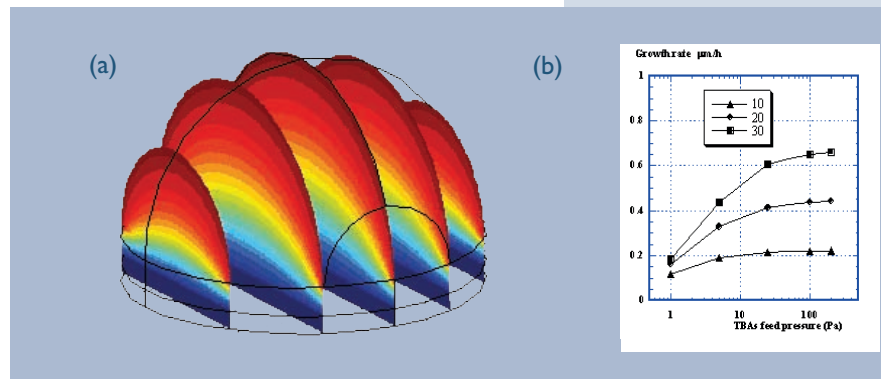


FIGURE 2: The COMSOL Multiphysics plot on the left (a) shows the gallium concentration in a nanowire. Figure 2(b) shows the wire growth rate for various source pressures for the arsenic and gallium, here referred to as TBAs (tertiarybutylarsine). Higher levels lead to a higher gallium concentration at the surface of the gold seed particle, resulting in a faster growth rate.

Commenting on these results, Prof. Stenström says, "At this time, our model deviates with experimental data by only a factor of two. When I say 'only,' I admit that in many situations that amount would be unacceptable, but in this case we think it is quite good given the limited amount of data we have for this process. Part of the reason for these deviations comes from the fact that we don't fully understand what is going on in the reaction, so we have to make a number of assumptions."

Prof. Stenström is familiar with COMSOL Multiphysics from previous work, and he was happy to use it for this application. "It's easy to create the geometry, set up the boundary conditions, and enter the physical data for the system. I was also able to enter my own expressions for the reaction rate, whereas other codes would require us to write our own equations in a much more cumbersome fashion. Further, COMSOL Multiphysics offers good plotting facilities and visualizes results very well. Overall, the package fits in well for problems in chemical engineering such as this." ■

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