Abstract - This paper investigates the modes of thinking that may be required to understand the concepts central to nanotechnology. Six senior scientists at a large Midwestern university were interviewed to uncover their way of thinking about nanotechnology. The semi-structured interviewers were coded and analyzed to identify the researchers’ underlying concepts, ideas, and ways of thinking about nanoscale phenomena. In addition to confirming that previously identified concepts such as self-assembly are important for understanding nanoscience, interviews also pointed out that the concept of “defect” has a whole new meaning in nanomaterials. System thinking was also identified as central to understanding the nanoscale world.

Index Terms: Epistemology, Nanotechnology

INTRODUCTION

The nanotechnology revolution, famously foretold by physicist Richard Feynman’s in his 1959 talk, “There’s Plenty of Room at the Bottom,” is now upon us. Nanotechnology research programs have sprung up everywhere and exciting new results of this research are being announced with greater and greater frequency. Most researchers working in this new interdisciplinary field recognize that doing work in the nano-scale requires a new kind of thinking. But what IS this new thinking? And how should this new way of thinking be passed along to students as we educate engineers to be able to contribute to the work that nanotechnology is building?

In order to answer these questions, we have begun to delve the way of thinking (or epistemology) of noted nanotechnology researchers.

METHODS

Email invitations to participate in the study were sent to senior researchers at a major nanotechnology research center at a large Midwestern University. Six senior faculty and expert scientists in the area of nanotechnology with backgrounds in Chemistry, Electrical Engineering, Materials Science, and Interdisciplinary Engineering volunteered to be interviewed.

The following are a sampling of interview questions related to the focus of this paper:

- What do you consider are the key concepts in your discipline that are related to nanotechnology?
- Are any of these concepts new in your field? How are these concepts different from other concepts?
- Why do you think these concepts are important?
- How did you learn about these concepts?
- How did you make sense of it?
- What models of thinking/mental models have you used to help yourself understand them (concepts)?
- What is making these concepts difficult?
- How do these concepts inter-relate?
- Why these concepts are characteristic of nanotechnology?
- Do you think there are threshold concepts that your students must know in able to grasp the new ideas related to nanotechnology in your area?

Interviews were transcribed and analyzed. Grounded Theory approaches were employed to analyze the data. Grounded theory is a theoretical framework in which themes and findings emerge directly from the data. Strauss and Corbin [1] described it as a systematic approach of data collection and analysis where theory is inductively derived from the study of the phenomenon it represents. The process of inductive analysis consisted of a process of identification of differences and similarities in the data, resulting in a set of categories or themes and their properties and interrelations [2]. Using these approaches we investigated how expert researchers make sense of nanoscale phenomena. In particular, we sought to determine commonalities existing
among specific concept and ideas related to nanoscale phenomena and strategies these experts employed for making sense of such phenomena.

**RESULTS**

The results of this study provide insight into what are the required concepts, ideas and ways of thinking required for understanding nanoscale phenomena. We first identify the prior knowledge required and particular ideas that take importance at the nanoscale. Then, we identify system thinking and its characteristics as the required ways of reasoning and sense making tools for understanding phenomena at the nanoscale.

**Prior Knowledge and Important Ideas.**

There was a common consensus among Dr. Summers and Dr. Bailey that a strong background in Physics and Chemistry are the required prior knowledge in order to understand nanoscale phenomena.

Dr. Summers: Okay? But I think fundamentally you need to have strong physics, chemistry, math background [that will] increase your ability to understand abstraction.

Dr. Bailey: Certainly I have not ever imagined that the fundamentals of physics and physical chemistry that I learned as an undergraduate, and then promptly forgot for the next couple of decades, would be so important when I got into this area where I'm working with engineers.

In particular, Dr. Kingston and Dr. Summers mentioned solid-state physics as additional training while Dr. Woodson, Dr. Summers, Dr. Kingston and Dr. Smith mentioned quantum mechanics.

Dr. Kingston: Right, so they are—so if you said to somebody, well, in a typical physics program, they've taken all the quantum mechanics courses, they've learned about solid state physics, at the very end of their Ph.D. program they might have now a course on what in physics you might call quantum statistical non-equilibrium quantum mechanics, which is like putting statistical mechanics, quantum mechanics, openness and non-equilibrium all into once package, and then you say, “Well, that’s what you need to know for nano.”

Dr. Summers: Well the primary tools I think for nanoscience, you need to have a good strong math background; you need to have a good fundamental physics background; and in particular the field of solid-state is a key one, and quantum mechanics is a key one. Because for electrical, optical, magnetic and thermal properties, those are all quantum mechanical and solid-state ideas, that are being manipulated.

Dr. Woodson: My advice is that they [students] ought to start with quantum mechanics first in the physics department and then decide where they want to go from there because quantum mechanics is fundamental to what nanoparticles do.

Particular classical ideas from these subject areas that become important at the nanoscale are the physical interactions that take place between molecules, and forces at the nanoscale.

Dr. Bailey: And I think that’s important to think about; all the physical interactions that take place between molecules. The van der Waals forces and the hydrogen bonding and the ionic attraction take on sort of a new meaning when they are multivalent; and multivalent, I mean there are multiple of these interactions.

Dr. Woodson: Well, so to do that one needs to understand the function of all the organic molecules and materials that are used in biology- in these areas that you mentioned and once you understand that you need to understand what the nanoscale will do to change the functionality, to improve it or broaden it or things like that, so that’s the challenge I would call the grand challenge for people working in nanotechnology is to understand what the role of the nanoscale is in these applications at some point in time.

Important new ideas or concepts particularly related to nanotechnology are the interesting materials that show different properties at the nanoscale that are size and/or shape dependent.

Dr. Summers: In my sub-area of looking at mostly electronic materials the primary point of nanotechnology is that as you go to smaller and smaller size scales of materials, the properties of electrons become fundamentally different, due to quantum mechanical constructs. The fact that they are confined to … small systems makes them have different answers for how they choose their energy, and thus it gives them different properties. So if you take a piece of silicon that is big, and you
ask what the electrons have as options for their energy—which is related to all their properties in the end—and you take that same piece and you scale it down sufficiently small, the electron is sensitive to the boundary of the crystal, the absence of the piece of silicon, and it reacts to that in a specific way that changes how the energies are distributed, and thus it gives different electron properties… So for me the key concept in my sub-branch of nanoscience is that as you go to smaller size scales, electron properties change; and we want to understand how to create structures at that size scale, so that we can get the properties we desire.

Dr. Woodson: Well, my understanding is that there are fairly large molecules that can be measured in the nanoscale that if they’re twisted in a certain way they will function a certain way and if they are done differently they’ll function differently so the size and shape of these particles seems to be very important.

The idea of self-organization was another concept that takes on particular importance at the nanoscale. This concept is tightly related with forces at the nanoscale:

Dr. Smith: Another area that is a theme is bottom-up self-organization or directed self-organization. So if you think about it from a manufacturing point of view, if you were going to build a nanoscale system what you would really like to do is take advantage of the relatively weak forces that now become relatively strong at that scale to self-organize structures. So you don’t have to go in and top-down to find everything essentially by carving things up, by etching and deposition. You can now do a little of that, but you can combine that with self-organization. And that’s a common feature in nanotechnology.

A new interesting and particular idea is that the concept of error at the nanoscale or smaller scales takes a different meaning.

Dr. Smith: The other thing that jumps out when I think about nanotechnology is that not only do the properties depend on scale, but you’re in a funny regime where if you make things a lot smaller, or smaller than what is generally considered to be the nanoscale, so say you’re working at the one nanometer and below level, so molecules. The concept of a defect doesn’t make much sense. I mean, you can have different handedness of the molecule, right and left handed. Or you can have different molecules. But the idea of a missing atom or some mistake in the way things are organized just doesn’t make a lot of sense. Statistically speaking, it’s not going to happen, you don’t have to worry about it. At the larger scale, say micron scale, all engineering materials and devices are loaded with defects. You can’t avoid them.

Dr. Summers provided us an example of how the concept of error has a different meaning at the nanoscale:

Dr. Summers: I have a whole lecture where I describe the growth of quantum dots. Again, if I were in graduate school, we wouldn’t have done that, because that was just a screw up in crystal growth, at the time. Right?... But then what happened is someone said, “But wait a second. If I do that, and I get these guys all the same size, then what I’m doing is providing a new material; germanium that’s small, that has different electron wave functions.”… And so the equations, they’re all the same equations, but now you’re saying, “Okay, I’m going to provide a sufficient amount of flux that the atoms are coming in quickly, and they’re moving around at temperature, and they agglomerate.” As opposed to providing them more slowly, where they move around and find nice clean lattice sites to do this leverage; a whole lot more than that. And before, that would’ve been a discussion in class of, “Oh, this is how crystal growth goes wrong.” Instead of growing planar and planar by layer, now you have this problem, and they grow in humps. And you don’t want the humps, you want layer by layer. Well, in fact, if you control that, then you instead have a new thing.

Ways of Thinking

Although many of the concepts related to nanotechnology are the same basic concepts that have been taught in the past, researchers, such as Dr. Bailey, have identified that one of the particular qualities for understanding nanotechnology is to understand how those concepts and principles interact as a system:

Dr. Bailey: That’s one of the interesting things about nanotech is because it’s complex systems, you can predict probabilities for what will happen, but there’ll be all these emergent properties if you do not. So I think that sort of the courses that people could benefit from, as we move into this era, are things like systems
Dr. Stone referred to this way of thinking as the ability to "put the story together":

Dr. Stone: They [students] learn pieces, but they don’t usually put it together in a big, like a story. I think that’s really what it is, is you kind of have to have a storyline.

In particular, gaining understanding of nanoscale phenomena requires understanding the different levels of a system. Dr. Stone explained it as follows:

Dr. Stone: But I think realistically what’s different is that you have to understand both surfaces and bulk or continuous materials. You have to understand the internal properties and the surface properties. And that has to be kind of in balance, because everything that we do at the nanoscale includes both. You certainly cannot ignore surfaces, so you need to have some understanding of what a surface is and what happens when you truncate a bulk material and create a surface.

For example, two of the main ideas related to nanoscale science and engineering that require thinking at different levels are the understanding of forces at different scales and understanding a different concept of defect. Stone described how it is required to think “like an atom or a cluster of atoms and molecules or surface at the atomic scale,” in order to be able to understand how different forces interact at different levels:

Dr. Stone: And then the self-organization is kind of a separate thing, but the reason that you can do self-organization is that you have these what are generally thought to be relatively weak forces at the macroscopic. But they become fairly strong forces at the nanoscale. They’re not strong enough—we’re not talking about covalent bonds and building crystals there, we’re talking more about Van der Waals or a secondary type bipole, dipole interactions, that sort of thing, where they’re relatively weak, which means that things will, if you give them enough thermal or vibrational stimulation, you can get them to move around and kind of gradually move towards some structure with some order.

Another example is provided by Dr. Bailey who explained how they have to start thinking in terms of atoms, molecules and then moving into nanostructures:

Dr. Bailey: Well so the concepts that I focus on, when I teach undergraduate organic, are mechanisms; mechanisms of how molecules interact... But you have to actually walk through atom by atom... We’re … at the very molecular level. And different disciplines focus at different levels. And so I think the physicists still have to focus on fundamental particles and how they operate; how they assemble; how they lead to emergence of the properties that are characteristics of molecules. Well we happen to, as organic chemists, function on the level of molecules; how single molecules interact. And so we focus on that for a year. And then it’s the next level, biochemistry, year three in undergraduate, where okay, now you have all these molecules, how do these molecules interact? And it’s biology at that level where you begin building nanosystems.

Dr. Stone also explained how it is required to think at different levels of a system in order to understand how the concept of self-organization of atoms in a nanostructure that can result in a different concept of defect:

Dr. Stone: But then also, that introduces another level of defect in that when you’re organizing these things with these weak forces, it’s pretty common that you’re going to have something missing... A missing particle or a particle that’s a little too big and that will cause a distortion around it, which will cause the next particle to go into the wrong place. So you typically have a fairly high what we would consider a defect density. It’s rare to get a million nanoparticles to organize themselves without a defect. Getting 10 or 100 may not be rare, but getting a million is rare. So this means that not only do you have to worry about atomic-scale defects, but you have worry about nanoscale defects as well, which would be defects associated with self-organization. So those are all features of the nanoscale that you don’t really have at the microscale. Those surface forces may still be important, but not at that level. And at the molecular scale, it’s different too. You can build very complex things without defects at the molecular scale.

Key characteristics of complex systems at the nanoscale that need to be identified are equilibrium versus non-equilibrium,
open versus closed systems, and distinction between homogeneous versus continuous versus discrete.

Dr. Kingston: I mean, typical quantum mechanics is limited to closed systems, but still students need to understand the fundamentals of quantum mechanics but then they need to expand on that. And the expansions that are necessary are dealing with open systems, dealing with systems that are out of equilibrium, and dealing with systems where the underlying material is not homogeneous but granular in atoms, and then do that for systems that might contain a million atoms so that makes the computation very challenging.

For example, Dr. Kingston, in the context of a transistor device, explained how systems cannot be considered in equilibrium:

Dr. Kingston: But as an electrical engineer I deal with systems that are not in equilibrium. I apply a voltage to my contacts of my device. That means on one end of the device the electrons are at a higher energy, potential energy, than in the lower end, at the other end of the device, and that potential energy is induced by an external battery, by an external energy source, and that drives the electrons in from one end through the device into the other end and somewhere energy is getting lost. That is distinctly not in equilibrium and you need to consider the various processes in which, number one, electrons move through the structure from one end to the next in one direction rather than in a closed system, and then there are these interactions.

Dr. Kingston also made an important distinction between open versus closed systems, and the importance of this distinction.

Dr. Kingston: The other thing that quantum mechanism typically does when it’s being taught is, either the systems are closed so you consider some finite domain and electrons or particles can’t get in or out, and they basically experience a hard wall sort of like they can’t get beyond a certain domain, you confine them, or you consider something that is called periodic, meaning you consider a finite domain, but then you assume that domain to be repeated in all directions. That’s called a periodic assumption. But either way none of these systems are, in a sense, truly open systems meaning you have a sort of a box in the middle of the device. Conceptually in that box it could stay connected to an infinite channel or an infinite pipe which can supply electrons and the other end of the device is also open and electrons can get out. So from a conceptual point of view a closed system and an open system are very different in their behavior. The mathematics are more complicated in an open system, and again, that feeds into dealing with a transport in the structure because you can’t get electrons in and out if you assume you have a closed system, really.

Dr Summers also emphasized the importance of open vs. closed systems but in the context of boundary conditions (i.e. lack or presence of confinement):

Dr. Summers: The most common idea is that as you go to a small size scale and provide the fundamental new boundaries to the material, properties change; all of them. [But] they change in different ways. Electrons react to that differently than atomic vibrations; those are phonons, and that’s what transfers heat in material. Okay? When you have something that’s got a hot side and a cold side, it’s the motion of atoms, correlated motion of atoms, that transfers the heat from the hot to the cold. Okay? And if you take a big, bulky thing—right?—it moves along with the heat equation, and we use an old-fashioned equation to solve that. If you go to very small nanowire structure, it doesn’t work the same way, because the atom vibrations field different answers, because of the lack of confinement. So each of these cases, it’s just a specific, fundamental, internal thing. Atom motion, electron choices, correlated atom motion—which is plastic deformation—they all change as you provide smaller structures and new boundary conditions.

Interviewer: So new boundary conditions would be a new idea? You mentioned also lack of confinement.

Dr. Summers: Yes. Lack of confinement or presence of confinement. Both. So sometimes it’s the lack of confinement that changes properties, and sometimes it’s the presence of a confinement. So in nanotechnology we specifically design structures that have very small elements that are confined between other elements, because again that changes how electrons interact.
Finally, Dr. Kingston also explained as important the distinction between systems that are homogeneous versus continuous versus discrete.

Dr. Kingston: And the third one that is critical it is homogeneous versus, say, continuous versus discrete. Most of semiconductor physics in the traditional sense is being done by assuming that you have a conduction band edge in a band where electrons can move freely... So it says, well, they are slightly modified from a traditional free electron mass, but with these two quantities you can basically compute anything you want. That means you can take a material and make it bigger or smaller. You wouldn’t know that there are actually atoms in this geometry. It’s just a continuum jelly. And most quantum mechanical simulations are even done in this model where they assume that everything is continuous underneath, and they describe it by something called plane waves.... There’s no concept of discreteness in this model. Well, but if you look at a real crystal, and a typical semiconductor crystal might be looking like a so called zinc blend crystal...

If you actually look at it from a one, one, one angle, from X, Y, Z looking from this angle you will see a completely different crystal because the overlap, the point overlaps are different... So the symmetry is important, and if the symmetry is important and you say, “Well, I’m going to make a nano device that’s only ten boxes of this wide,” then it’s going to matter how I’m going to chip my ten boxes in which crystal direction. So crystal direction and the discreteness—well, crystal direction is important and you can argue, well, I still don’t need to know about atoms, but at the end if you’re down the line of making something five nanometers wide, let’s say that’s ten atoms, it’s not 11 it’s ten, and it’s not 12 it’s ten, right? And it matters. And then if you have a finite crystal and an edge you might have a dangling bond and that might have a hydrogen atom sitting on it, which might change the chemistry, which you would never capture or even dream of arguing about in the continuum model because you can subdivide however you like. So to me these are the three key elements [non-equilibrium, openness, and discreteness], assuming that you know about quantum mechanics, and solid state physics, and all that, right? But these are the key elements that make up nanotechnology in my realm.

DISCUSSION

The results of this preliminary study confirm previous findings identified as big ideas of nanoscience. Concepts such as properties and forces at the nanoscale and the idea of self-assembly were concepts identified by most of the participants. However, participants also pointed out that not all materials have interesting properties at the nanoscale, but just few materials show those properties (i.e. quantum dots). A new concept identified that takes particular importance at the nanoscale is the concept of error. This idea takes a new meaning because what it could be thought as an error in the microscale may be simply seen as an emergent property of a material at the nanoscale.

On the other hand, this study also provides new insights. As some participants explicitly stated, in order to understand nanotechnology one must understand complex systems. Learning concepts at the nanoscale requires a new understanding of systems at different levels. One must have an understanding of the overall pattern of what is happening in a system and simultaneously understand what is going on with the phenomena at the nano- and bulk levels. Thinking about systems requires an awareness of the conditions of emergence such as non-equilibrium, openness, and discreteness.

Knowledge about how expert researchers think about nanotechnology can be used to inform curriculum and contribute to the education of future nanotechnologists. Thus this line of research has both theoretical and practical implications.

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