Engineering Research Towards Societal Benefit

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The Center for Nanoscopic Materials Design

Key Discoveries and Insights Generated by MRSEC

- There are prospects for using MRSEC-developed techniques to direct the self-assembly of NbO_2 nanodots on TiO_2 single crystal substrates.
- An array of NbO_2 nanodots on a TiO_2 surface could serve as the foundation for a bio-nano scaffold that assists in understanding wound healing, the progression of atherosclerosis in arteries, and tumor cell invasion.
- Consideration of the societal and ethical implications of nanotechnology (SEIN) has been instrumental in identifying the NbO_2 / TiO_2 opportunity and defining a graduate engineering degree project to explore the opportunity.
- Assembly of an *interdisciplinary team* of social and natural scientists to guide this SEIN-based MRSEC research project has created an intellectual *trading zone*.
- Fruitful exchange within the *trading zone* has been facilitated by creation of a common reduced language (a *creole*) that allows team members with different intellectual backgrounds to *Collaborate and Iterate* on the vision for a two year, graduate engineering research project (a masters degree).

Collaborations

The concepts and initiatives presented here have been made possible through:

- A 1 year, $100,000 NSF NIRT Award on the Societal and Ethical Implications of Nanotechnology (SES-0210452).
- The NSF MRSEC Award to the Center for Nanoscopic Materials Design at the University of Virginia (DMR-0080016).
- A NSF / DOD REU Site Award on Nanoscale Design and Control of Self-Assembled Materials (EEC-0244436).
- A NSF Careeer Award to Rosalyn Berne on Ethics and Belief Inside the Development of Nanotechnology (SES-0134839).

The team is also reaching out to the University of Virginia's Institute for Practical Ethics (www.virginia.edu/ipe/) to further develop the *Collaborate and Iterate* model of SEIN-based nanotechnology research.

State-of-the-Art

The University of South Carolina: www.cla.sc.edu/cpecs/nirt/

2001 NSF NIRT (1 year, $175,000), 2002 NSF NIRT (4 years, $1.3 million):

- Philosophy of science: Understanding how something so small can be seen and manipulated into reliable technologies;
- Depiction of nanoscience: Understanding how the nanoscale can and should be visually depicted and simulated (visually and in writing) in everything from microscopy to science fiction, the arts and literature;
- Concepts and ethics of risk: Understanding the human and environmental risks of nanoscience and how to address public concerns, ranging from toxicity to fears of possible runaway technology;
- Public perception: Understanding how nanoscience should be conveyed to journalists and the public at large.

Rice University: www.ruf.rice.edu/~cben/

2001 NSF NSEC, Center for Biological and Environmental Nanotechology

- Study the environmental and health consequences of nanoscale materials.
- Develop new nanomaterials that interact with aqueous systems at multiple length scales, including interactions with solvents, biomolecules, cells, whole-organisms, and the environment.
- Consider whether their methods or materials might contribute to health or environmental hazards.

UCLA: 2002 NSF NIRT (4 years, $1.49 million):

- To study how newly acquired knowledge about nanotechnology makes its way from laboratory to marketplace.
- To estimate the impact of nanoscale science and technology research upon firms' entry into and success in the marketplace.
- To analyze academic scientists' involvement in commercialization and how that affects their scientific productivity and teaching.
- To develop extensive databases on small nanotechnology startup firms.

NSF: Workshops on the Societal Implications of Nanoscience and Nanotechnology (2000 - 2003).

Other:

- Societal Implications of Nanoscience and Nanotechnology (Kluwer Academic Publishing) 2001.

Significance of Insights, Commercial Applications

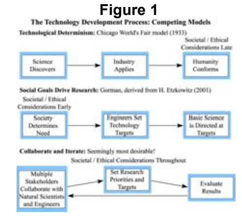
Development of this bio-nano scaffold should appeal to a range of commercial sectors. In addition to health care, the underlying technology developed here can likely be applied to chem-bio hazard and environmental monitoring systems. Intellectual property disclosures are planned in the near future as an early step towards commercial application.

Results to Date

Using considerations of the Societal and Ethical Implications of Nanotechnology (SEIN) to motivate project activity

- Activity centers around Robin Catalano's masters degree in Materials Science and Engineering that considers SEIN throughout its duration.
- The project is co-advised by a cognitive scientist, Mike Gorman, and a materials scientist, James Groves. Collaboration of this type (i.e. among diverse stakeholders) occurs within a *trading zone* - a location where social scientists, ethicists, engineers, and natural scientists work together at the 'bleeding edge' of technology development to generate advances endorsed by society.
- SEIN considerations enter every research discussion. To balance SEIN with nanotechnology science and engineering (NSE) aspects of the project, the team follows a *Collaborate and Iterate* model of technology development (Figure 1).

Figure 1



- A record of the SEIN + NSE process employed here is being recorded by Jeff Shrager for future reference.
- To facilitate effective communication within the *trading zone*, the team has established a common reduced language (a *creole*) that allows exchange of knowledge among team members with diverse intellectual backgrounds.
- In the *creole*, reaching the summit of a mountain signifies development of the understanding necessary to explain a major scientific unknown (Figure 2).

Figure 2

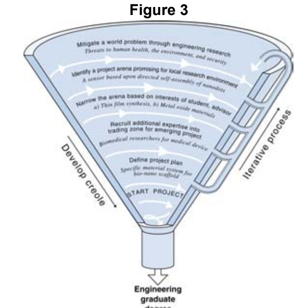
- Injection of SEIN into the process has shaped the project from the outset. For instance, the project started by asking the following question: How can this project contribute to mitigation of one or more recognized world ills (Table 1)?

Table 1

World Ills	Symptoms
Air Quality Degradation	Climate change Ozone layer depletion Particulate matter Acid rain
Soil Pollution	Persistent organic pollutants
Water Pollution	Unsustainable fisheries Marine pollution Groundwater contamination
Disease	HIV / AIDS Cancer Heart Disease
Unsustainable Development	Biodiversity loss Desertification Overpopulation
Poverty	Illiteracy Inadequate housing Gender disparity in education
Hunger / Thirst	Insufficient sanitation Food insecurity Limited clean water supply Child mortality
Terrorism	Chemical, biological, and radiation hazards

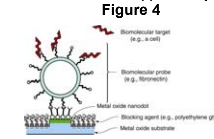
- Having agreed to motivate the project through consideration of world ills, a set of self-imposed constraints have sought to focus attention on a specific, reduced set of research challenges manageable during a single masters degree project (Figure 3).

Figure 3



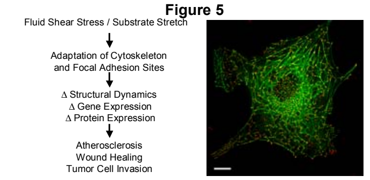
- Consideration of SEIN has initiated a move towards creation of a bio-nano scaffold of broad applicability (Figure 4).

Figure 4



- Rather than reaching to create a bio-nano scaffold of broad applicability (too ambitious for a single masters degree project), a scaffold useful for the basic research of Brian Helmke and Colin Choi in the local environment has been selected as the first mountain to climb (Figure 5).

Figure 5



Nanopatterned extracellular matrix surfaces will provide critical tools for designing spatial cues to engineer structural dynamics and cell behavior.

- Before initiating specific investigations, streams between the trailhead and mountain summit have been identified and stepping stones across each have been scouted out (Table 2).

Table 2

Streams	Stepping Stones
1. Are there metal oxide systems (substrate / film combinations) that might island during growth due to small lattice mismatch?	Y. Liang, et al. (2001). P. R. Markworth, et al. (2001). Y. Gao, S. A. Chambers (1996).
2. For metal oxide systems that might island, can selective biomolecule adhesion be induced (i.e., molecule A to substrate, molecule B to nanodot)?	R. Michel, et al. (2001a). R. Michel, et al. (2001b). M. Kosmulski (2001).
3. When exposed to this bio-nano scaffold, are cells viable for the duration of subsequent experiments?	See Table 3.
4. Can the metal oxide islanding self-assembly process be directed using MRSEC processes?	See Figure 6 (Results from MRSEC graduate student Yingge Du).

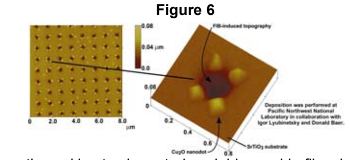
- Having identified these obstacles on the trail, the team decided that a bridge could reasonably be built only across the first stream during this first masters thesis project.
- Bridges over the other identified streams are being built elsewhere within the MRSEC or will need to be built later as part of follow-on activity.

Table 3

Metal Oxide	Isoelectric Point	Crystal Structure	Lattice Parameter (A)	Biocompatibility
V_2O_5	2.5	Orthorhombic	11.52, 3.56, 4.37	Probably
Nb_2O_5	4.0	Orthorhombic	6.18, 29.2, 3.93	Yes
ZrO_2	4.4	Monoclinic	5.14, 5.21, 5.31	Yes
Mn_2O_3-	4.7	Cubic	9.48	Probably
PtO_2	5.0	Hexagonal	3.08, 4.19	Probably
MnO	5.5	Cubic	4.44	Probably
TiO_2: Substrate candidate	6.0: M. Kosmulski (2002)	Tetragonal: Y. Gao, S. A. Chambers (1996)	4.59, 2.96: Y. Gao, S. A. Chambers (1996)	Yes: S. Kothari, et al. (1995), V. Faust, et al. (2002)
NbO_2: Nanodot candidate	7.3: M. Kosmulski (2002)	Tetragonal: Y. Gao, S. A. Chambers (1996)	4.77, 2.96: Y. Gao, S. A. Chambers (1996)	Probably: R. Kurrat (1998), H. Matsuno, et al. (2001)
Y_2O_3	7.6	Cubic	10.6	Probably
Fe_2O_3-	8.1	Hexagonal	5.01, 13.7	Probably
Fe_2O_3-	8.1	Cubic	9.4	Probably
Al_2O_3-	9.0	Hexagonal	4.85, 13.3	Yes
ZnO	9.0	Hexagonal	3.25, 5.21	Yes
CdO	10.6	Cubic	4.7	Probably not
MgO	11.0	Cubic	4.22	Probably

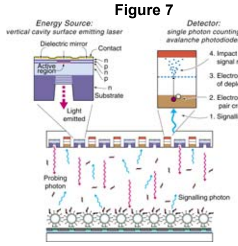
- In Table 3, a metal oxide's isoelectric point appears critical for selective biomolecule adhesion, crystal structure and lattice mismatch could be important for metal oxide directed self-assembly, and biocompatibility is important for cell viability.
- Based on the SEIN + NSE process employed here, the team has identified NbO_2 on TiO_2 as a promising material system candidate for bio-nano scaffold development.
- Recent MRSEC results have demonstrated the ability to use FIB patterning to direct metal oxide nanodot growth (Figure 6).

Figure 6



- Currently working to characterize niobium oxide films by sputter deposition using XPS (chemistry) and XRD (crystal structure) analysis techniques.
- In the future, this work could lead to development of bio-nano-based sensor array systems as shown in Figure 7.

Figure 7



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Project Publication

M. E. Gorman, J. F. Groves, and R. K. Catalano, "Collaborative Research into the Societal Dimensions of Nanotechnology: A Model and Case Study," *Technology and Society Magazine, IEEE*, submitted (2003).

Integration of Research and Education

Graduate

- Materials Science and Engineering and MRSEC graduate student Robin Catalano is performing the research that forms the core of this initiative. Not only is she conducting state-of-the-art nanotechnology science investigations but also she is being exposed to SEIN concepts and considerations on a daily basis.
- All graduate students within the MRSEC program are being exposed to the developments of this initiative through the Center's regular Journal Club series. Both Gorman and Groves have given talks during which SEIN concepts have been presented and debated.
- MRSEC graduate students have examined SEIN through a seminar discussion led by Prof. Deborah Johnson, a member of UVA's Division of Technology, Culture, & Communications, and the university's Institute for Practical Ethics.

Undergraduate

- As part of the NSF MRSEC-affiliated REU site, undergraduate students participating during the summer of 2003 enrolled in a 2 credit seminar course on nanotechnology ethics. The seminar was organized by Carolyn Vallas and led by Rosalyn Berne.

Next Research Steps

Specific Project Investigations

- Synthesize NbO_2 nanodots on TiO_2 substrates (Bridge #1), possibly at Pacific Northwest National Lab (PNNL), working with Igor Lyubinetsky and Donald Baer. The work is likely to include mapping of process space where NbO_2 forms (vs. Nb_2O_5).
- Verify ability to direct the self-assembly of NbO_2 growth on TiO_2 (Bridge #4), possibly at PNNL.
- Investigate selective biomolecular adhesion to NbO_2 and TiO_2 (Bridge #2).
- Establish cell viability in presence of NbO_2 / TiO_2 scaffold (Bridge #3).

Broader Link of SEIN into Engineering Research

Mike Gorman has submitted a 2003 NSF NIRT proposal, requesting an expansion of this SEIN-based research. Two new MRSEC / SEIN projects are proposed as a continuation of this bio-nano scaffold effort and new connections to other institutions and segments of the nanotechnology community.

Nathan Swami and Carolyn Vallas have submitted a proposal to NSF's Research Experience for Teachers program. Gorman and Groves will guide K-12 teacher development of modules that encourage students to consider government investment in nanotechnology.