

RESEARCH QUESTION

Does stochastic surface behavior affect the effective properties of nanoparticles?

RESEARCH OBJECTIVES

1. Study the stochastic behavior of surface stresses on the effective properties of nanowires. For this we need:
 - To use Matlab as an investigative tool.
 - Reproduce and validate fundamental methodology (based on perturbation method)
2. Utilize this research as a foundation in class to introduce key concepts in statistics.

CAN YOU SEE ME NOW?

100 nm 90 nm 80 nm 70 nm 60 nm 50 nm 40 nm 30 nm 20 nm 10 nm 1 nm

Nanobelt (80nm) Z.L. Wang, GT
Au-FePt nanocomposites (30 nm) Sellmyer, Nebraska
Magnetic nanostructures (8 nm) Liu, UC Davis
Microbial electric nanowires (2 nm) Logan, PennState

Quantum effects Nanoelectronics Novel structures

TEM SEM HPC Why nano? Why now? Z.L. Wang C. Singh P. Yang

A Fundamental Difference at the Nanoscale Geometric: the characteristic length (grain or particle size) of the microstructure.
Physical: the amount of grain boundaries per unit volume.

What is the effect of surface properties on the effective behavior of nanoscale devices?

Specifically, how do stochastic events occurring on the surface impact the surface behavior?

INTRODUCTION

This research attempted to examine the stochastic behavior on the effective properties of nanowires. Two published papers were studied, analyzed and replicated as theoretical model.

The results/findings of this research will be an essential part in the implementation of a new formulation developed by the research advisor, Prof. Remi Dingreville. The product of this research (mechanical model) will account for the surface effects for nanoparticles.

BACKGROUND INFORMATION

Microstress estimate of stochastically heterogeneous structures by the functional perturbation method: A one dimensional example (Eh Altus, 2006)

Solving for Var(u)

$$u^{(n)} = \sum_{i=1}^n c_i^{(n)}$$

With these conditions:

$$c_i^{(n)} = \text{const}(x_i - x_{i-1}) \text{const}(x_i - x_{i+1}) \times \int_{x_{i-1}}^{x_i} \int_{x_i}^{x_{i+1}} \text{const}(x_i - x) \text{const}(x - x_{i+1})$$

$$c_i^{(n)} = -\text{const}(x_i - x_{i-1}) \text{const}(x_i - x_{i+1}) \times \int_{x_{i-1}}^{x_i} \int_{x_i}^{x_{i+1}} \text{const}(x_i - x) \text{const}(x - x_{i+1})$$

$$c_i^{(n)} = -\text{const}(x_i - x_{i-1}) \text{const}(x_i - x_{i+1}) \times \int_{x_{i-1}}^{x_i} \int_{x_i}^{x_{i+1}} \text{const}(x_i - x) \text{const}(x - x_{i+1})$$

Fig 1. Y-axis is a function of the (n-1) and (n+1)th elements

Fig 2. Y-axis is a function of the (n-1) and (n+1)th elements

Fig 3. Y-axis is a function of the (n-1) and (n+1)th elements

Fig 4. Y-axis is a function of the (n-1) and (n+1)th elements

-Altus devised an explicit method in calculating characteristics of a non-uniform, stochastic field of a one dimensional heterogeneous structure

-The analytical result permits an insight to morphology related effects on displacement and stress fields

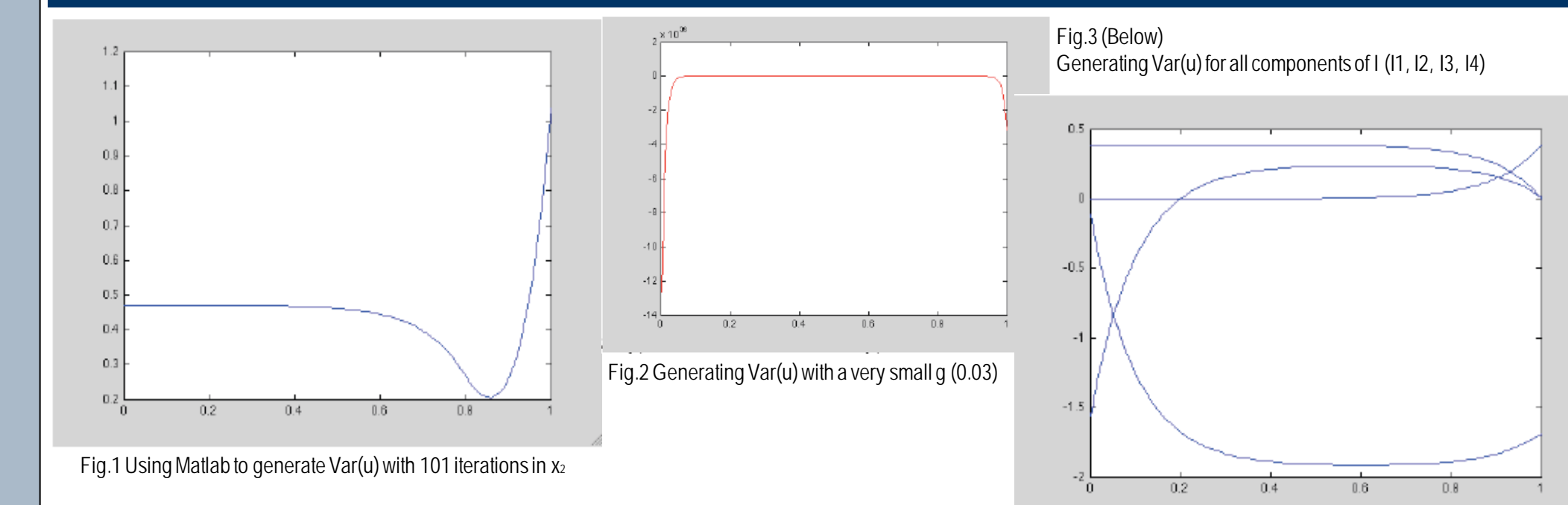
In order to establish mathematical perspective and to acquire experience in understanding engineering principles and theories related to stochasticity and nanomechanics, two published research papers were studied and analyzed: Altus 2006 and Altus, Bar On 2006.

The main purpose of this initial investigation is to adapt and validate the methods and strategies used by the two authors mentioned. A Matlab code was generated based on the computational model presented.

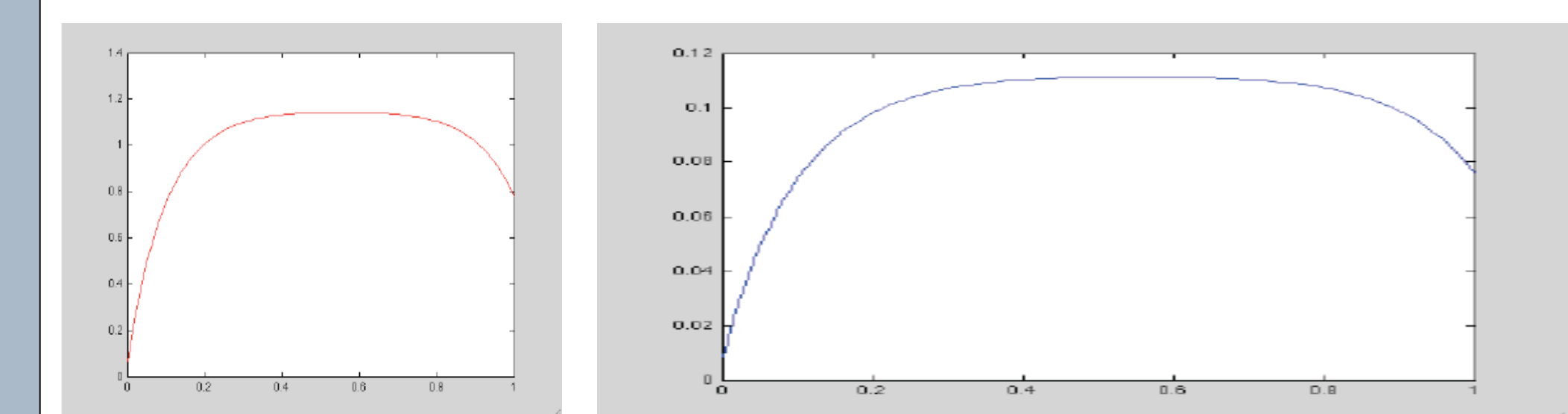
RESEARCH PROCESS



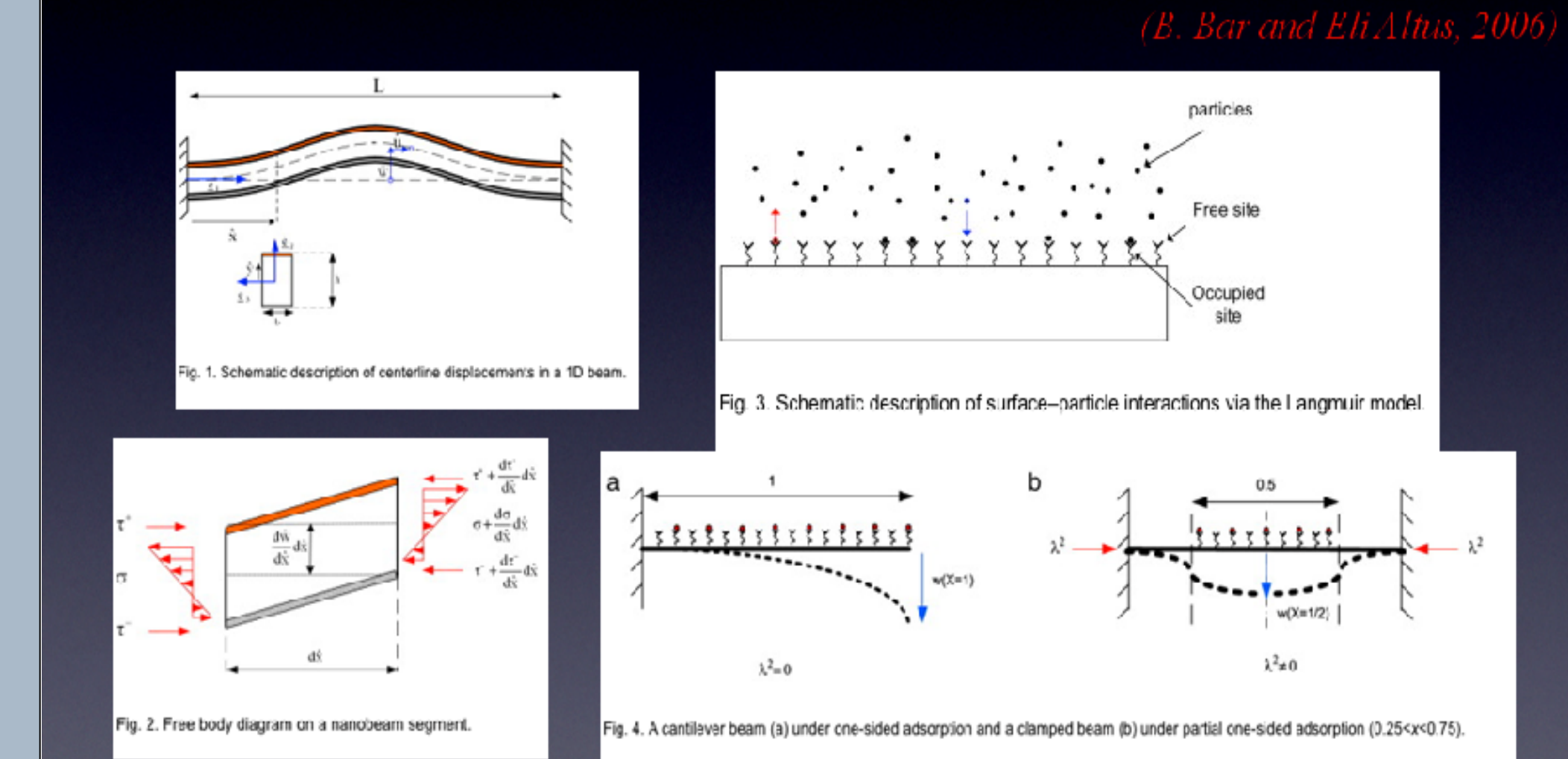
REPLICATION RESULTS



Figures 1, 2 and 3 shows the progression of the Matlab program codes of the formula Altus (2006) used to find Var(u). The figures below were generated when all the iterations were put together (I1+I2+I3+I4)

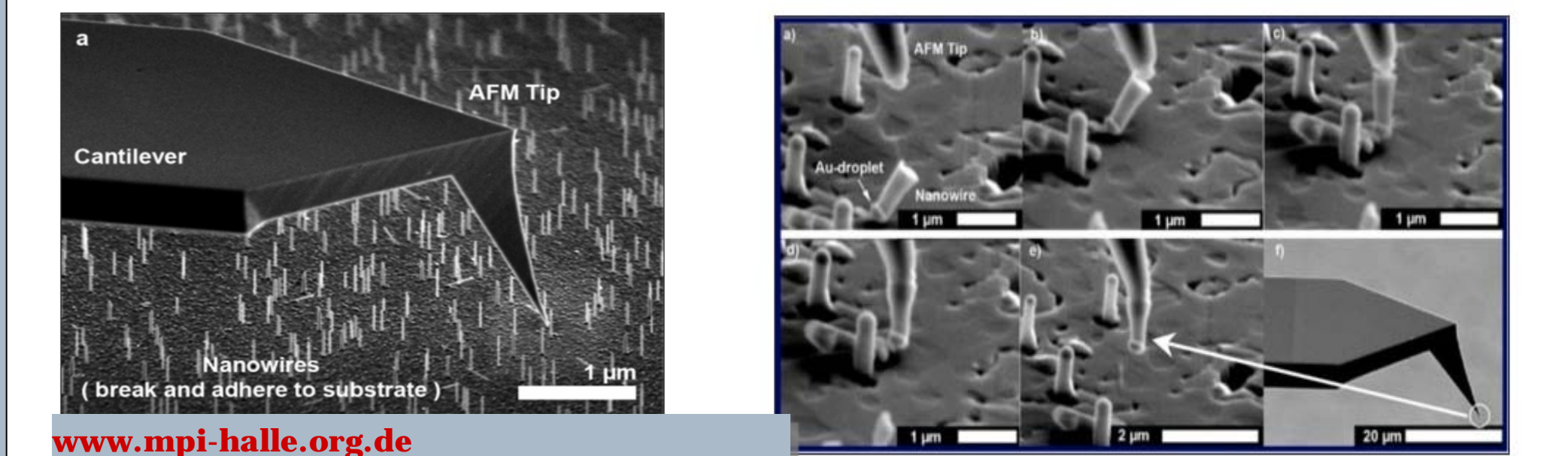


Stochastic surface effects in nanobeam sensors



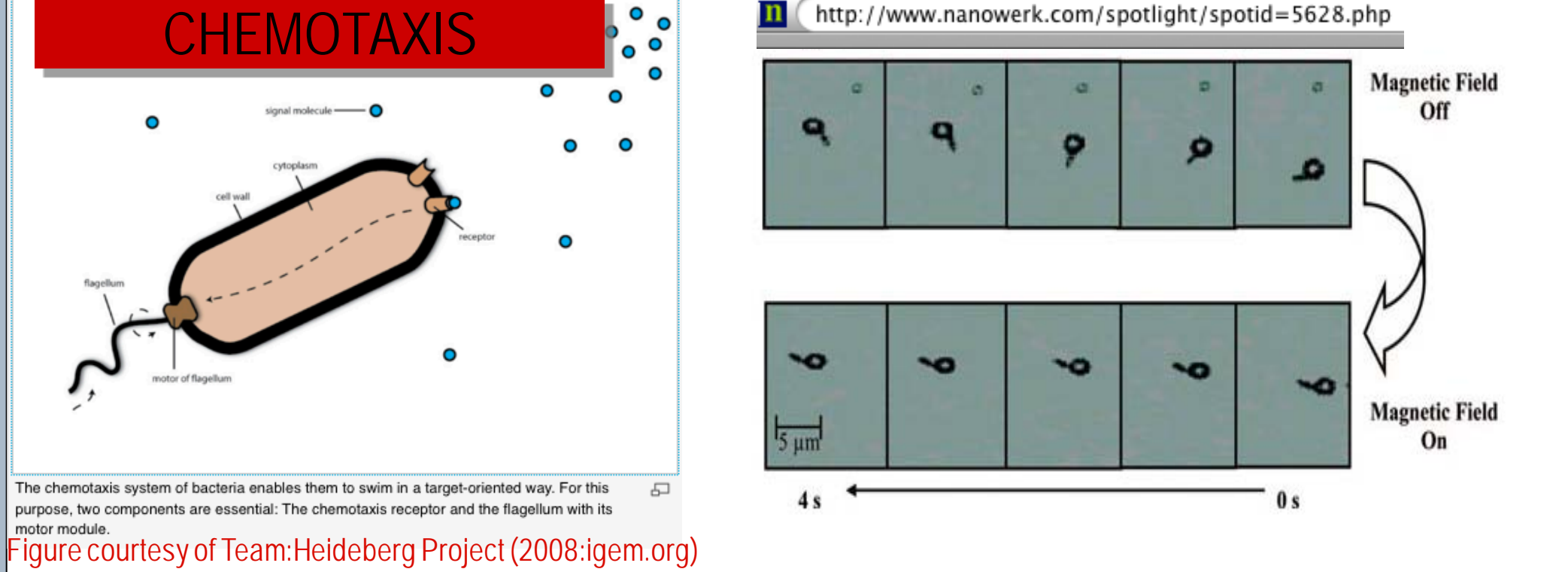
APPLICATIONS

One method of harvesting nanowires:



Nanomaniipulation sequence for the attachment of an up-side-down nanowire onto an AFM tip: a) Mechanically, some nanowires are broken off the substrate by the movement of an AFM tip; b) A nanowire that lies on the substrate surface is brought into contact with the AFM tip; c) The nanowire is moved into the desired position; d) Welding of the nanowire to the AFM tip by electron beam induced contamination; e) Retraction of the AFM tip; f) Cantilever with tip and welded nanowire assembled to be used as a TERS probe.

Observing movements of chemotaxing bacteria consuming metallic ions:



CONCLUSION

Based on the resultant mechanical formulation of this research in conjunction with the mechanical model of the effects of buckling on nanowires (separate study), it is possible to quantitatively and qualitatively characterize the mechanical behavior of such devices. This type of approach will enable a faster integration of such devices in relevant technological applications.

FUTURE PERSPECTIVE

1. Sustain the computational momentum to validate perturbation method for surface effect
2. Establish the mechanical model of stochastic effects for nanostructural devices
3. Produce lab results to reproduce the theoretical at a bigger length scale.
4. Publish research
5. Incorporate some of the concepts used into classroom to teach some key materials in statistics

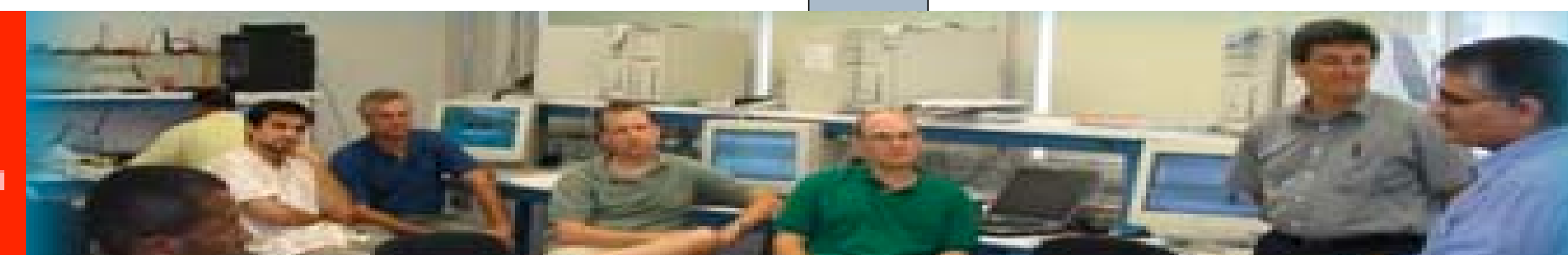


The National Science Foundation SMART Program Research Experience for Teachers

ACKNOWLEDGMENTS

NYU-Poly Mechtronics Lab
Prof. Vikram Kapila, Project Director
Prof. Remi Dingreville, REsearch Advisor

Mechtronics Lab Techies:
Jared, Parth, David
Special mentions: Nichole, Ankur, Leo, Muhammad, and all the people who helped in their own ways



SMART
Science and Mechtronics Aided Research for Teachers :
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This material is based upon work supported by the National Science Foundation under an RET Site Project with Grant #: EEC-0807286