#### Algae Biofuels: Designing Biofuels We Can Believe In

Joel L. Cuello, Ph.D. Department of Agricultural and Biosystems Engineering

#### Scope

With Energy as the NAE Grand Challenges theme, our studies aim to achieve the economical and sustainable large-scale production of algae biofuels, while maximizing the potential of its production-biorefinery process to approach carbon neutrality as much as possible. Past and current studies have focused on algae photobioreactor design with incorporation of reuse of waste CO2, reuse of wastewater and the use of available solar radiation through the use of a fiberoptic-based solar concentrator.



Participants (COE and UA)

Gene Giacomelli (CEAC)

Murat Kacira (CEAC)

**Robert Freitas** 

Kimberly Ogden

#### Central questions to be answered or issues to be addressed:

To achieve the economical and sustainable large-scale production of algae biofuels, while maximizing the potential of its productionbiorefinery process to approach carbon neutrality by designing integrated closed-loop systems that reuse waste CO<sub>2</sub>, wastewater, biomass residues and waste heat, and which makes use of any coupled or generated energy such as syngas, biogas or thermal energy or available solar radiation.



#### Knowledge/expertise

Photobioreactor design and scale up Algae culture optimization

#### Collaborators' Knowledge/expertise

Supercritical CO<sub>2</sub> extraction Algae oil characterization Algae biodiesel characterization and testing Algae molecular biology



#### Previous and ongoing work

CO<sub>2</sub> sequestration using algae culture

Algae production in photobioreactor equipped with solar concentrator Algae photobioreactor design and scale up based on hydrodynamic

Hydrogen gas production from algae culture through manipulation of photosynthetic electron transport system

Modeling of biogas generation from duckweed biomass Use of algae in photobioreactors for wastewater treatment



## Potential research direction/projects

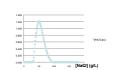
Coupling pyrolysis to algae production system Pilot scale of an integrated algae production and biorefinery system Integrating algae production system to an electric power plant Supercritical CO<sub>2</sub> extraction of fatty acids from algae biomass











Vessel Dispersion Number **Bodenstein Number** 

**Axial Dispersion Coefficient** 

Reynold's Number

Mixing Time

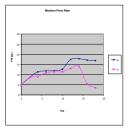
Algae Productivity



Photobioreactor hydrodynamic conditions









#### **Arid Lands Sustainable Bioenergy Institute ALSBI**

Co-Directors: Don Slack, ABE UA & Ron Richman, Innovative Technology **Development Center** 

#### Scope

Mission: Apply strengths in plant sciences, water resources engineering, agricultural engineering, energy and sustainable engineering practice, to develop technologies and a local base of industry to meet the increasing challenges of providing renewable bio-energy within the constraints of our fragile and evolving environment.



#### **CROPS**

#### **TOOLS & RESOURCES**

CONTROLLED PILOT SCALE BUSINESS

#### **RESEARCH**

#### **SWEET SORGHUM**





**GUAYULE** 





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GAE

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FACILITIES  *Acreage 1,500 Acres  *Controlled Water Quality  *Tillage	ENVIRONMENT AGRICULTURE •Greenhouse •R&D platform for crop production	•Biodiesel production	DEVELOPMENT  Industry liaisons  Commercial- ization	/ FABRICATION SHOP •Electronic •Equipment fabrication
equipment GENOMICS	BIOREACTORS	DUDIEICATION	ENVIRONMENTAL	SYSTEM ANALYSIS
Regulation of gene expression     Genetic     Engineering	•Bench Scale •Pilot Scale •Photo- bioreactors	•Filtration •Filtration •Centri- fugation •Distillation	ENVIRONMENTAL RESEARCH LABORATORY •Water Quality Analysis •Wastewater/ Reclaim Water Sources	STSTEM ANALYSIS  *Computer Simulation  *Economic Analysis

#### **PARTICIPANTS**

#### **LESQUERELLA**

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COE

Dennis Ray (PLS) Kim Ogden (CHEE) Judy Brown (PLS) Greg Ogden(CHEE) Mike Ottman(PLS) Perry Li (AME) Don Slack (ABE) Kumar Ramohalli (AME) Joel Cuello (ABE) Mark Riley (ABE) Peter Waller (ABE) **Bob Freitas (ABE)** Randy Ryan (AES) Colin Kaltenbach (AES) Ursula Schuch (PLS) Gene Giacomelli (ABE) Leslie Gunatilaka (OALS)

**CALS** 

IRRIGATION

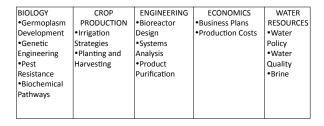
#### COS

Mike Cusanovich (ARL &Biochem)

Pinal Energy, Maricopa, AZ Sweet Ethanol, LLC, Tucson Grecycle, Tucson **US Bureau of Reclamation** San Carlos Apache Tribe **Bosque Engineering, Tucson APS Energy Innovative Technologies Development Center, Tucson** 

INDUSTRY/GOV'T

INSTRUMENTATION



#### **PRODUCTS**

LIQUID FUELS	BIO-	SPECIALTY	BIOMASS	
(Biodiesel, Jet Fuel, Biooils, Ethanol)	CHAR	PRODUCTS	FUELS	







#### **RESULTS**

We have developed or adapted harvesting and crushing equipment for sweet sorghum. We grew 7 acres of sweet sorghum in 2008 and delivered ~12,000 gallons of juice to Pinal Energy for fermentation. We have also been producing biodiesel from used cooking oil at a pilot plant at the Campus Ag. Center. We have produced "biochar" by pyrolizing sweet sorghum bagasse and other cellulosic materials at the Red Rock Ag. Center.



#### The ATLAS Center: Transportation Systems **Planning, Management and Operations**

#### Scope

The ATLAS (Advanced Transportation and Logistics Algorithms and Systems) Center at the University of Arizona organizes research and education in transportation systems. The Center directly addresses the NAE Grand Challenge to restore and improve urban infrastructure by focusing on ways to improve the utilization of and reduce the congestion in the nation's transportation system. Programmatic areas in the Center include transportation operations and traffic control, transportation simulation and planning models, roadway safety, and transportation sensor and decision support systems. The ATLAS Center supports faculty in Engineering, and faculty in other disciplines and in other universities.



#### 1. Central Issues to be Addressed

- 1. To conduct basic research and system development for advanced technologies, information systems, and methods for transportation and logistics management.
- 3. To collaborate with agencies and industries and to assist in the implementation of this research and development.
- 5. To enhance education and technology transfer activities that enhance the state of the practice in transportation and logistics management.

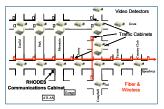
#### 3. Research Opportunities

- 1. Testing new vehicle-infrastructure communication systems to inform drivers of potential road hazards and to assist drivers to improve traffic safety and operations
- 2. Understanding of integrated transportation system dynamics in urban areas, covering: (a) land use, (b) personal activity patterns and resulting travel, (c) traffic dynamics, and (d) air quality and vehicle emissions. Models can be used to describe system evolutionary behavior.
- 3. Developing a comprehensive simulation platform to consider real-time traffic and transportation management strategies, such as traffic control, traveler information, pricing, transit operations, pedestrian movements, etc.
- 4. Designing new sensor systems to monitor vehicle and personal movements, in order to identify behaviors of interest and to improve modeling realism.
- 5. Developing decision support systems to help traffic engineers optimize traffic signal timing and ramp metering to improve traffic flow.
- 6. Identifying methods and algorithms to improve the quality of transportation data.

#### 4. Funding Opportunities

- National Institute of Standards and Technology (NIST)
- National Science Foundation
- US Department of Transportation (University Transportation Centers program)
- Arizona Department of Transportation
- Industry collaboration for real-time and long-term transportation management

#### 2. Previous and On-going Work



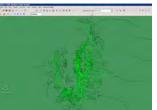
Living Laboratory for Transportation Technologies (City of Tucson)



MILOS Adaptive Ramp Metering Operational Test (ADOT)



Remote Sensing of Traffic Activities at Border Crossings (US DOT)



Large-Scale Traffic Simulation using DynusT (US DOT)



System (ADOT)



Simulation of Emergency Evacuation of Cardinals Football Game (ADOT)

#### 5. Expertise Gaps

- Interface of transportation systems with the environment
- Interface of transportation systems with energy systems
- Advanced sensor systems for vehicle and person detection and monitoring
- Transportation and driver safety
- Infrastructure management and long-term planning

#### 6. Participants and Partners

- Pitu Mirchandani (Director, SIE), Larry Head and Wei Lin (SIE), Yi-Chang Chiu and Mark Hickman (CEEM)
- Affiliated faculty in College of Engineering and other Colleges
- Arizona State University and Northern Arizona University
- US DOT (FHWA, RITA), NSF, NCHRP, ADOT, TxDOT, MAG, PAG, Maricopa County, City of Tucson, City of Tempe, etc.
- The University of Arizona and the College of Engineering
- Collaborations with many other universities, research centers, consultants, etc.



#### **School of Sustainable Engineered Systems**

# Biologically Inspired Nano-Manufacturing (BIN-M)

#### Science Foundation Arizona Customized Project

#### PIs:

- Anthony Muscat, Chemical and Environmental Engineering, UA
- Megan McEvoy, Biochemistry and Molecular Biophysics, BIO5 Institute, UA
- Masud Mansuripur, College of Optical Sciences, UA

#### **Graduate Students:**

- Amber Young, PhD candidate, College of Optical Sciences, UA
- Sam Jayakanthan, PhD candidate, Biochemistry and Molecular Biophysics, UA
- Rahul Jain, PhD candidate, Chemical and Environmental Engineering, UA

#### Other Researchers:

• Zhengtao Deng, Postdoctoral Fellow, ChEE & Optical Sciences, UA

#### Cost Share (other than core ERC funding):

Science Foundation Arizona, ASM, SEZ-LAM

## **Objectives**

- Minimize cost of materials, energy, and water to fabricate nanoscale devices using bio-based strategy
- Exploit homogeneity, mild reaction conditions, and specificity of active biological molecules
- Grow 3D structures to achieve scalable architecture
- Employ additive, bottom up patterning methods

## **ESH Metrics and Impact**

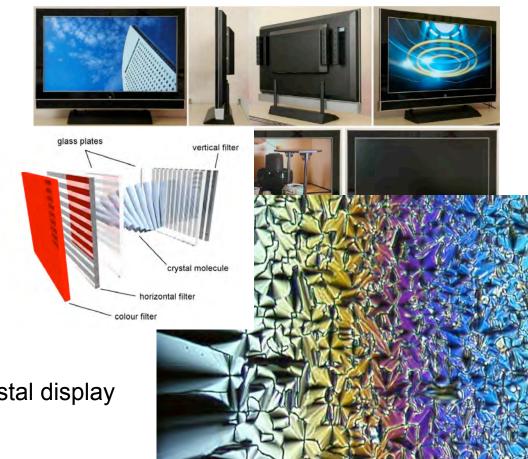
Sustainability metrics				
Process	Water l/bit/masking layer	Energy J/bit/masking layer	Materials g/bit/masking layer	
Subtractive 32 nm*	3.3x10 <sup>-10</sup>	1.5x10 <sup>-12</sup> EUV	2.9x10 <sup>-16</sup>	
Additive	3.6x10 <sup>-13</sup>	9.2x10 <sup>-17</sup>	1.8x10 <sup>-19</sup>	

<sup>\*</sup>D. Herr, Extending Charge-based Technology to its Ultimate Limits: Selected Research Challenges for Novel Materials and Assembly Methods. Presentation at the NSF/SRC EBSM Engineering Research Center Review Meeting: February 24, 2006.

## **Self Assembled Structures**

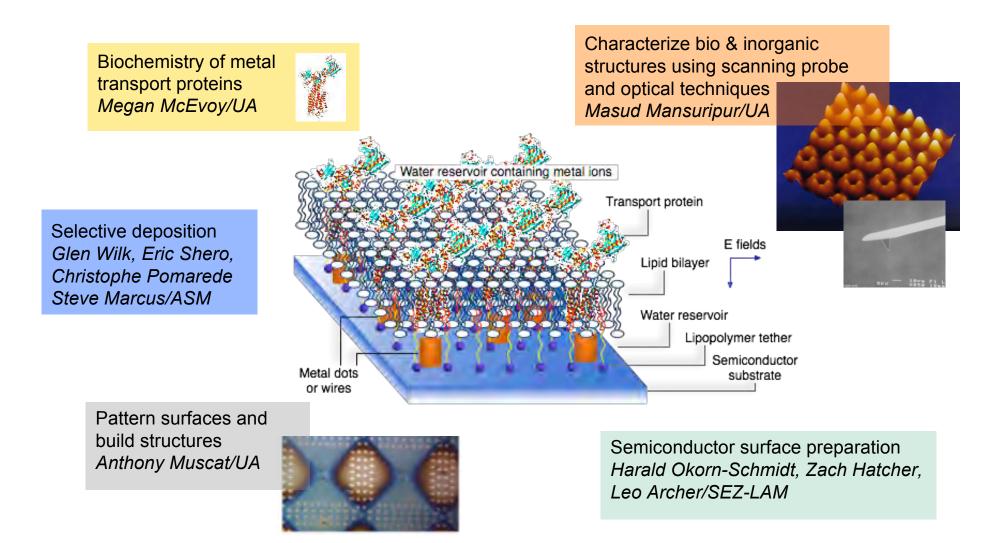


DNA



Liquid crystal display

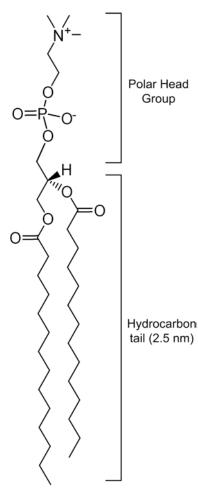
## **Process Goal: Deposit Array of Metal Dots**



## **Lipid Bilayer Formation**

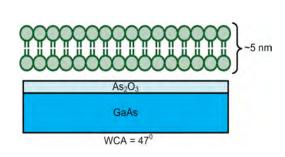
## (Mask in Traditional Subtractive Process)

- Lipid bilayer deposited on substrate by vesicle fusion method
- Non polar hydrocarbon tail of DMPC is estimated to be 2.5 nm long
- Vesicle fusion
  - Droplet of vesicle placed on a substrate, where it adsorbs, breaks up and spreads, forming a bilayer
- AFM is an ideal tool to study the characteristics of these membranes since it can generate high resolution images

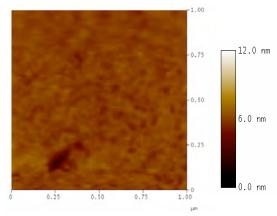


1,2-Dimyristoyl-*sn*-Glycero-3-Phosphocholine (DMPC)

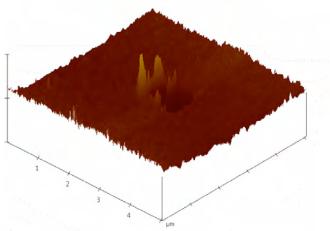
## Lipid Bilayer formed on GaAs



Schematic of lipid bilayer on As<sub>2</sub>O<sub>3</sub> terminated GaAs

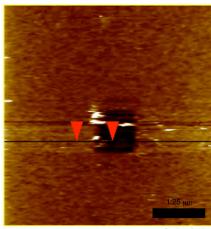


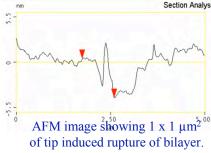
AFM image of lipid bilayer on As<sub>2</sub>O<sub>3</sub> terminated GaAs surface.



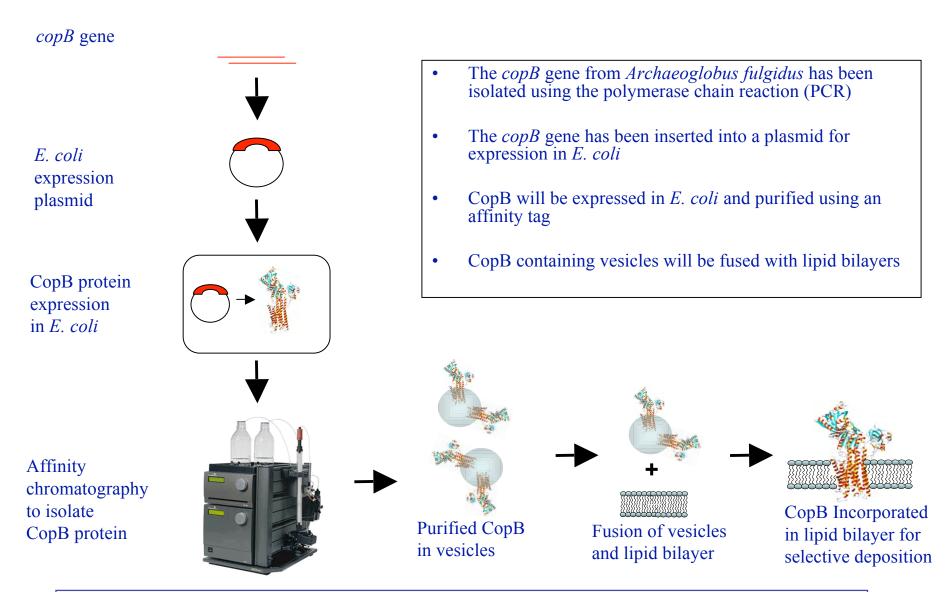
3D view of the tip induced rupture.

- Bare GaAs surface:
  - RMS roughness <0.4 nm over 1x1 μm² region.
- Bilayer on As<sub>2</sub>O<sub>3</sub> terminated GaAs
  - AFM confirmed the formation of lipid bilayer.
  - RMS roughness <0.2 nm over 1x1 μm² region.
  - AFM height image and corresponding cross section analysis of the tip induced rupture process. The height difference indicated by markers is ~5nm.

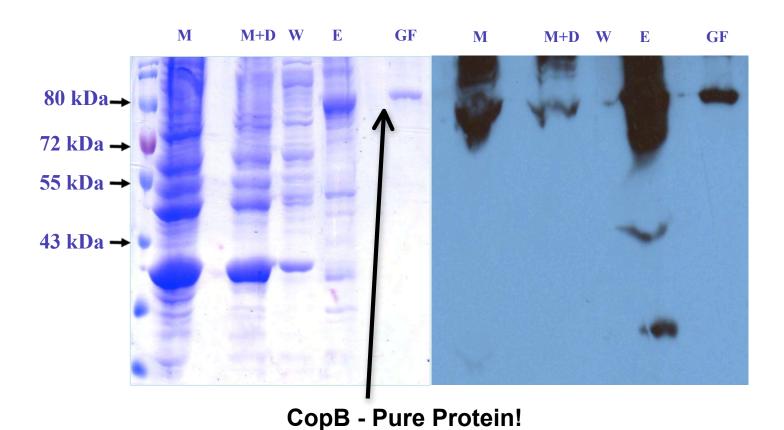




## **Preparation of CopB**

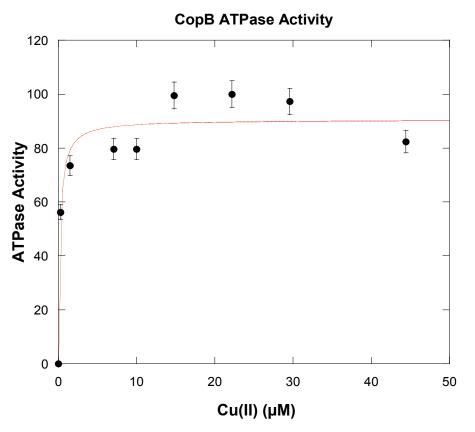


## Transport Protein Synthesized and Purified



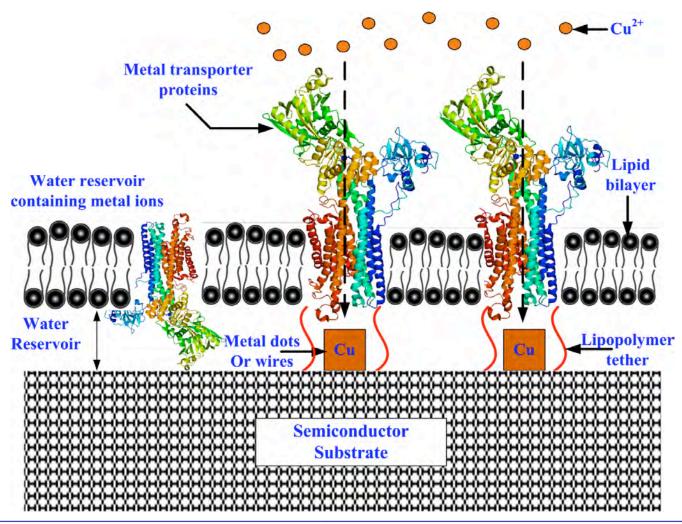
SDS-PAGE gel of a Histidine tagged protein prep performed on a Ni(II) affinity column (Left), western blot of the same gel (Right). Lanes: M – total membrane protein, M+D – detergent solubilized protein, W – wash with 30 mM imidazole, E – Elution with 400 mM imidazole, GF – sample purified through gel filtration (Sephacryl S-300).

# Activity & Copper transport by A.fulgidus CopB

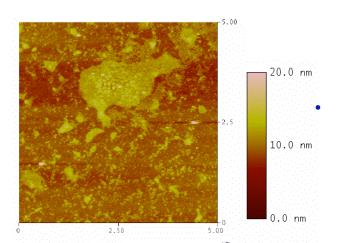


- Enzyme activity as determined by plotting the rate of release of inorganic phosphate as a function of copper concentration.
- The data was fit to the Michaelis-Menton kinetics to measure the maximum velocity at which the enzyme hydrolyses ATP.
- The Michaelis constant was determined to be  $K_m$ =0.20  $\pm$  0.08  $\mu M$ .
- The enzyme was found to have a maximum velocity of  $V_{max} = 90.48 \pm 3.6$ , where 100% = 6.22 nmol/mg. of Enz/h.

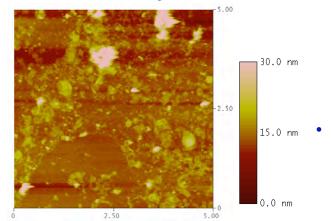
## **Integration**



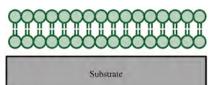
## Copper Transport through A. fulgidus CopB



AFM height image showing copper islands on HF etched GaAs surface 5-15 nm high without the use of protein

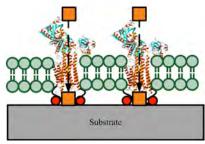


AFM height image showing copper islands on HF etched GaAs surface 20-50 nm high using protein



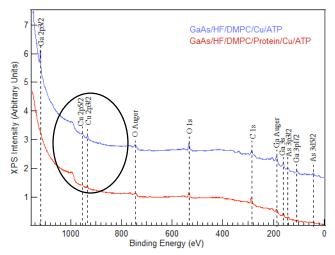
#### HF treated GaAs surface:

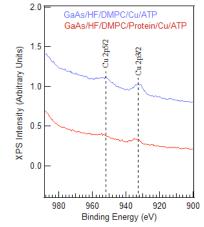
- Addition of ATP to the already formed lipid bilayer
- Addition of Cu<sup>2+</sup> for verification of deposition of Cu without the proteins
- Cu deposited on the substrate due to a non continuous bilayer or contamination while washing the bilayer



#### HF treated GaAs surface:

- Incorporation of protein in the lipid bilayer followed by ATP addition
- Addition of Cu<sup>2+</sup> to deposit as Cu<sup>0</sup> on the substrate through transporter proteins
- Cu deposited on the substrate





XPS data showing copper deposition on HF etched GaAs surface with and without protein

# Industrial Interactions & Technology Transfer

- Presentation on liquid and gas phase cleaning of high mobility substrates to SEZ
- Jeremy Klitzke from SEZ visiting scientist at UA
- Surface modification development with ASM and LAM/SEZ projects

## **Future Plans**

#### Next Year Plans

- Liquid and gas phase cleaning of high mobility substrates
- ALD film nucleation on high mobility substrates
- Find conditions for maximum activity and thereby enhance Cu(II) transport
- Study stability and activity of *A. fulgidus* CopB in different lipid compositions
- Solve the crystal structure of the transporter using X-ray crystallography
- Demonstrate chemically patterned surface
- Incorporate proteins into the lipid bilayer
- Check compatibility of proteins in different lipid molecules
- Characterize proteins and structures using q-dots

#### **Long-Term Plans**

- Develop characterization techniques for nanostructures
- Demonstrate patterned nanostructures over cm length scale

# Publications, Presentations, and Recognitions/Awards

- "Biologically Inspired Nano-Manufacturing Using a Cu(II) ATPase" Poster presented at The 22nd Protein Society Symposium, July 18th, 2008, San Diego, CA. Presented by Sam Jayakanthan.
- "Structural and Functional Characterization of the Copper Transporting P1B-ATPase CopB from *Archaeoglobus fulgidus*" Seminar presented at the Biological Chemistry Program Journal Club Feb 5th 2009. Presented by Sam Jayakanthan

## Compressed-Air Energy Storage Systems for Stand-Alone Off-Grid Photovoltaic Modules

#### Scope

The design of systems capable of efficient energy storage is critical to the complete utilization of energy derived from solar-powered photo-voltaic (PV) units. As a small-scale, low-cost, alternative to current storage-systems (pumped hydroelectric systems, electrochemical modules, and large-scale underground compressed air storage systems), we propose a low-maintenance, environmentally-benign energy-efficient compressed-air energy-storage module to be used in conjunction with PV units.



PV module

#### **Problem Statement**

Examine the viability of using small-scale **compressed-air** modules as energy-storage systems in conjunction with stand-alone, photo-voltaic (PV) systems, for **off-grid** power delivery

- >Low-cost, low-maintenance environmentally-benign, high-efficiency isothermal compression system.
- >Off-grid alternative to the large-scale compressed air powered energy plants.
- > Can be specifically tailored to power individual household and commercial units and household appliances.

#### Previous and ongoing work

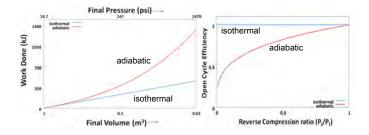
Ongoing work has focused on designing a prototype that can be customized for powering individual residential appliances.

Towards this end, we have designed an

ISOTHERMAL SINGLE-STAGE HYBRID COMPRESSOR/MOTOR UNIT

Advantages of an Isothermal Compression System

- · Ideal efficiency
- Can be tailored to completely utilize energy produced by stand- alone PV panels

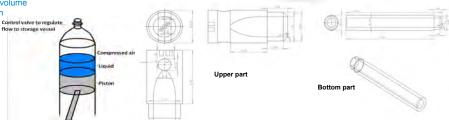


#### **Key Features of the Prototype**

- Hybrid compressor/motor single-stage design
- o minimize number of moving parts
- o Light duty (~ 60 rpm)-reduction in losses due to friction
- Electronically controlled air regulator in synchronization with the crank-shaft that controls the motion of the piston
- > Effective cooling system for isothermal compression/expansion
- o maximize efficiency, by operating at near quasi-static conditions
- o multiple fin-structure to promote thermal conduction

#### > Liquid 'Piston'

- o reduction in dead volume
- o decrease in friction



#### Potential research direction/projects

- > State of the art computational modeling and optimization methods for guiding
- · design of prototype
- · materials selection
- · reliability, safety and risk analysis

#### Knowledge/expertise gaps

- > Efficient energy recovery from compressed-air
- > Designing customizable units depending on the needs of the user
- > Materials issues (identifying the ideal fluid with desirable thermal, viscous and chemical properties)

#### **Funding opportunities**

NSF Sustainable Energy Program

DOE Office of Energy Efficiency and Renewable Energy (EERE)

Science Foundation Arizona (SFAZ)

Arizona Research Institute for Solar Energy (AzRISE)

#### Participants (COE and UA)

Krishna Muralidharan (MSE) Pierre Deymier (MSE) Larry Head (SIE) George Frantziskonis (CEEM) Samy Missoum (AME)



## STORAGE OF RENEWABLE ENERGY USING CAES

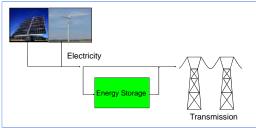
#### Scope

Utilization of renewable energy such as solar and wind energy is essential to secure the sustainability of economy and environment. A great challenge for maximizing the utilization and efficiency of renewable energy is the storage of energy. The research investigates different aspects of compressed air energy storage (CAES) in order to develop safe, efficient and cost-effective methods for storing renewable energy.



#### **Problem Statement**

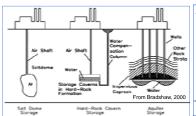
Different methods are available for storing energy, including compressed air energy storage (CAES), pumped hydro storage, thermal storage and battery storage. For the utilization of renewable energy, which is essential to secure the sustainability of economy and environment, the challenge is how to safely, efficiently and cost-effectively store the energy.

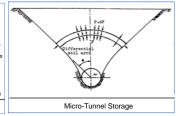


#### Previous and ongoing work

#### **≻**Geotechnical safety related to underground CAES

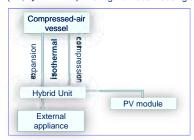
This project studies the geotechnical safety of potential methods for storing compressed air underground and intends to develop safe and cost-effective compressed air storage methods.





#### Compressed-Air Energy Storage Systems for Stand-Alone Off-Grid Photovoltaic Module

This project examines the viability of compressed-air storage modules in conjunction with stand-alone, off-grid photo-voltaic (PV) systems for powering individual housing units.

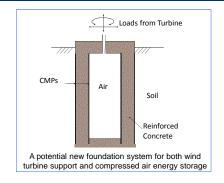


#### Knowledge/expertise gaps

- > How to increase the efficiency of air generation and utilization for CAES?
- > How to safely and cost-effectively store compressed air at different scales?

#### Potential research direction/projects

- >Development of cost-effective underground CAES system for different scale storage
- ➤New foundation system for both wind turbine support and compressed air storage
- >Development of efficient air generation and utilization system for CAES



#### **Funding opportunities**

NSF Sustainable Energy Program
DOE Office of Energy Efficiency and Renewable
Energy (EERE)
Science Foundation Arizona (SFAZ)

Arizona Research Institute for Solar Energy (AzRISE) Private Companies

#### Participants (COE and UA)

(in alphabetic order)

Muniram Budhu (CEEM)

Pierre Deymier (MSE)

George Frantziskonis (CEEM)

Kevin Lansey (CEEM)
Krishna Muralidharan (MSE)

Krishna iviuralidharan (IVISE)

Joseph Simmons (MSE)

Ben Sternberg (MGE)

Lianyang Zhang (CEEM)



SCHOOL OF SUSTAINABLE ENGINEERED SYSTEMS

## **Charge Generation and Transport in Nanoheterogeneous Materials**

B.G. Potter, Dept. of Materials Science and Engineering

#### Scope

The proposed program would establish a coordinated research initiative to develop a science-based understanding of charge formation and transport phenomena unique to nanostructured inorganic and molecular hybrid materials and composites. Guiding principles for the design and synthesis of these systems, evolving from this thrust, would directly impact the development of new energy conversion and environmental technologies based on these materials, including third-generation photovoltaics, fuel cells, high energy density batteries and capacitive storage systems, and heterogeneous catalysts. Research underway within UA and the College represents a strong nucleus of expertise from which to grow a unique University-wide competency and international reputation with broad impact to renewable energy, environment, and sustainable resource management.



#### **Motivation**

The evolution and transport of charge carriers within nanophase inorganic and molecular-hybrid materials systems is central to the successful realization of new material strategies for energy conversion, energy storage, and environmental applications. The interplay between interfacial and quantum-scale phenomena within nanoassembled composite architectures, for example, plays a critical role in these high surface area systems.

Despite sustained research effort, often focusing on specific applications, charge management still represents a key factor limiting the successful application of nanocomposite materials in these technologies.

UA/COE research could serve as the focal point for a center of excellence in this area with the potential for significant contribution to established national objectives in energy and environment.

#### Strategy

Establish core competency in nanophase electronic and optoelectronic materials and phenomena.

An integrated portfolio of program elements would connect intrinsic materials synthesis and property study to device-level performance.

- √ Novel thin film synthesis and nanoassembly (PVD, CVD, solution based film deposition, directed assembly)
- Integrated structure-property characterization including nanotopology, surface structure (e.g. SEM/TEM, scanning probe), intrinsic material functional properties (optical, electronic) and device-level performance (e.g. conversion efficiencies, charge/ discharge characteristics, catalytic yield)
- <u>Computational modeling</u> Available tools address multiple length scales/phenomena: FE, FD (charge transport); MC, MD (molecular assembly); DFT/TD-DFT (interfacial processes, charge trapping, excited state behavior)

#### **Existing Expertise and Research Activity**

Ongoing research within the College of Engineering and the new School of Sustainable Engineered Systems exists in each of these primary thrusts, including new materials synthesis and nanoassembly strategies, nanostructure and property characterization, and multiscale modeling of materials structure and charged species behavior. The efforts listed below represent examples of such work with potential impact on the proposed research theme. These could serve as a foundation upon which to enhance our base of expertise and develop new capabilities to attract funding in the area.

#### Research Efforts Include:

✓ Ge-ITO nanocomposites and nanostructured transparent conductive oxide (TCO) thin films for photovoltaics and integrated electronics: (Potter, MSE)

√ Nanoscale electronics via directed assembly of biological templates (microtubules) (Deymeir, Raghavan, MSE).



✓ Photonucleation of II-VI semiconductor quantum dots in molecular hybrid hosts (Loy, MSE/Chem; Potter, MSE)



- ✓ Nanostructures for heterogeneous catalysis and processes (Chem Eng.)
- √ In-situ CVD process analysis (Schrader, Chem Eng.)



✓ Density Functional Theory computation: including excitation paths, point defect and interfacial structure analysis (Corrales, MSE.Chem).



- ✓ Carbon nanotube-based conductive composites (Corral, MSE)
- ✓ Multi-length scale modeling of molecular assembly (Deymeir, Muralidharan, MSE; Corrales, MSE/ Chem)
- $\checkmark$  Polymer hybrid membranes for fuel cell applications (Loy, MSE/Chem).



✓ Photopatterned deposition of oxide and hybrid materials. (Potter, MSE; Loy, MSE/Chem).

✓ USIF (Seraphin, MSE)

#### Potential research direction/projects

An integrated research effort addressing both charge generation mechanisms and transport phenomena in nanostructured systems would require assessment of current capabilities and efforts to establish opportunities for leveraging expertise.

A potential structure for the formation of a unique expertise base could include organization around application (e.g. energy conversion, storage, optoelectronics) or materials systems (inorganics, organics, hybrids) with cross-cutting themes in fundamental phenomena (charge generation, transport processes).

Given the existing activities in material synthesis/testing and computational modeling, projects seeking synergism between these efforts should be pursued through integration of modeling (structural evolution/electronic phenomena) with nanostructural design and characterization.

#### **Funding opportunities**

The proposed activity impacts a broad range of interests, both fundamental and applied. Depending upon specific focus and team composition, funding opportunities for both single/multiple PI projects and center-level programs are anticipated from public and private sectors (e.g. DOE/BES and DOE/EERE, NSF, DARPA, AFOSR, SFAz, Research Corporation), in addition to partnerships with industry (Global Solar, General Plasma, Inc., Sion, etc.).

#### Participants (COE and UA)

In addition to the existing projects and personnel listed on the left, other research efforts and capabilities exist within the College and University, including:

- ✓ ECE (Nanostructured Si for PV: Melde, Potter)
- √ Optical Sciences (Nanotemplated surfaces and interfaces: Norwood)
- √ Chemistry (Excitonic organic PV: Armstrong)
- ✓ Keck Center for Nanoscale Structure and Dynamics



**School of Sustainable Engineered Systems** 

#### **Modeling and Management of Distributed PV** Generation, Storage, and (Smart) Grid

#### Scope

Solar energy resources are geographically distributed and dependent on the changing weather, which makes their direct control extremely difficult and requires storage units. The goal of this research is to design and develop integrated simulation, optimization, economic, and risk models, which will allow us 1) to obtain a robust and most economical mixture of capacities from conventional generation and PV generation, as well as storage while meeting reliability requirements against fluctuating demand profiles and weather conditions and 2) to evaluate various operational decisions. This work will be further extended to smart grid and demand management.



NAE Grand Challenges: Modeling and Management of Solar Energy System (To Make it More Economical)

#### 1. Central Issues to be Addressed

- 1. To reduce carbon dioxide created from traditional fossil fuels when burnt and make our environment healthier, providing an energy share from renewable sources (e.g. sunshine, wind, water, bio-fuel) is critical.
- 3. Major challenges associated with solar (focus of this research) generation
  - Geographically distributed and uncontrollable (dependent on the changing weather)
  - · Storage units are additionally required (save energy for night (short-term); save energy for peak season (long-
  - Interface with grid, smart-grid (emerging), and other sources (fossil, wind, water, bio-fuel)
- 3. Research Goal: design and develop integrated simulation, optimization, economic, and risk models, which will allow us to 1) obtain a robust and most economical mixture of various generation capacities as well as storage capacities while meeting reliability requirements against fluctuating demand profiles and weather conditions and 2) evaluate various operational decisions (e.g. store energy vs. sell it to the grid)

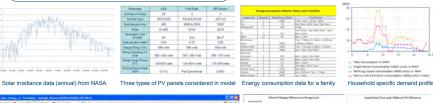
#### 3. Potential Research Direction

- 1. Fundamental systems engineering tasks of stating the problem, identifying stakeholders, discovering the stakeholder requirements, sensitivity analyses, and risk management. Risk management will identify, analyze and respond to perceived risks associated with the proposed project.
- 2. Development of a comprehensive simulation and optimization model considering various renewable sources (sunshine, wind, water, bio-fuel) as well as various storage techniques (compressed-air-energy-storage, batteries, super-capacitors, pumped hydro).
- 3. Modeling the above system as a multi-stage stochastic optimization problem, where one considers designing the storage system over a period of time with possibility of capacity expansion in later stages, as solar power becomes more accessible. We will devise novel methodologies and algorithms to solve this problem.
- 4. Finding optimal utility company strategies in the absence of current information and investigating how delayed information affects the optimal strategies.
- 5. Investigating and studying smart-grid, which will be 1) interactive with consumers (e.g. automatic metering) and markets, 2) self-healing and adaptive to correct problems before they become emergencies (e.g. outrage), 3) optimized to make best use of resources and equipment, and 4) predictive to prevent emergencies ahead
- Development of hardware (storage, generator, sensors)-in-the-loop simulation

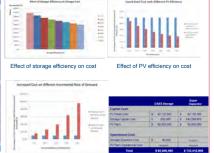
#### 4. Funding Opportunities

- Science Foundation of Arizona (Collaborative proposal with ASU/Tucson Electric Power (TEP) is pending)
- Theoretical work for Department of Energy; National Science of Foundation (unsolicited; solicited on energy)
- Practical work for major utility companies in Arizona (TEP, APS, SRP)
- Partnership with local industry (e.g. SOLON) for potential projects
- Leverage our relationship with Association of State Energy Research and Technology Transfer Institutions

#### 2. Previous and On-going Work







Developed flexible simulation/optimization model in AnyLogic Software

Effect of future demand growth on cost Comparison between CAES and SC

#### Advanced power systems (potential collaboration

with ECF or ASU)

5. Expertise Gaps

- Sensor network for monitoring demand (individual house), generation, storage (potential collaboration with ECE)
- Hardware technologies (PV, CAES, supercapacitor) (potential collaboration with MSE, Physics, Optics, or industry)
- Smart-grid and intelligent-grid

#### 6. Participants and Partners

- Young-Jun Son (SIE): Simulation-based Planning and Control
- Ferenc Szidarovszky (SIE): Dynamic Economic Systems
- Terry Bahill (SIE): Risk Management and Systems Engineering
- Guzin Bavraksan (SIE): Stochastic Optimization
- Larry Head (SIE): Dynamic Systems
- AzRISE (Joe Simmons, Ardeth Barnhart, Meredith Aronson)
- Arizona State University (Policy Analysis and Smart Grid)
- Association of State Energy Research and Technology Transfer Institutions (David Terry)
- Bill Henry at TEP (Data and Model Validation)



#### **School of Sustainable Engineered Systems**

#### **Integrating Entrepreneurship in Engineering**

#### Scope

Educating engineers to recognize the commercial potential of research discovery is a precursor to entrepreneurial activity including startup companies and technology licensing. The NAE Grand Challenges will require a strong foundation in economics, financial engineering, risk assessment, marketing, and project management to produce sustainable solutions.



## Entrepreneurship: a key component towards solving the Grand Challenges

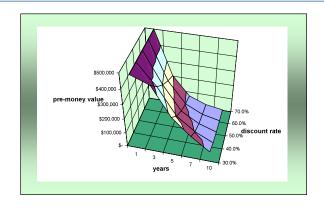
"Throughout the Grand Challenges Summit, speakers, panelists and audience members said over and over again that meeting the 14 grand challenges is going to require more than engineering and technology. It's also going to require driving forces in the form of public will, policy shifts and entrepreneurial activity."

## The Engineering Management Program Promotes Entrepreneurship Education

"The (NAE) panelists would like to see engineers and entrepreneurs working more closely together, and they would also like to see entrepreneurship skills taught in engineering schools." The EMG program integrates entrepreneurship into its engineering curriculum and has strong ties with the highly ranked McGuire Entrepreneurship Program in the Eller College of Management. Optimizing quality driven solutions to grand challenges in a chaotic environment of risk and reward confirm the importance of Systems Engineering.

#### Potential research direction/projects

Improving the success rate of new technology commercialization will require analysis and modeling to aid researchers overcome the enormous hurdles from discovery to economic viability to minimize early stage venture risk by integrating a Systems approach to include market potential, manufacturability, risk assessment, and financial engineering.



#### **Funding opportunities**

Integrating Engineering & Entrepreneurship is a major objective of the Kaufmann Foundation and the Thomas R. Brown Foundation. NSF funding is also possible via IGERT proposals.



#### Participants include:

M. Arnold

J. Hunter

F. Szidarovszky

J. Liu

McGuire Center for Entrepreneurship Office of Technology Transfer



**School of Sustainable Engineered Systems** 

#### MITIGATING DAMAGES TO THE NATURAL AND BUILT ENVIRONMENT FROM **GEOHAZARDS**

#### Scope

Natural and man-made geohazards have caused billions of dollars damages to the natural and built environment and loss of lives annually. Geohazards include earthquakes, floods, landslides, volcanoes, avalanches, tsunamis, debris flow, land subsidence, earth fissures, slope stability, mudflows, rockslide, erosion, and movement of glaciers and ice sheets

Grand Challenges and Theme: Infrastructure, Resources, Energy, Environment & global climate change



Muniram Budhu, Professor, Civil Engineering & Engineering Mechanic

#### **CENTRAL ISSUE**

HOW TO ASSESS, DESIGN AND MANAGE ENGINEERED SYSTEMS TO REDUCE THREATS TO HUMANS, MITIGATE DAMAGES TO THE NATURAL AND BUILT ENVIRONMENT FROM GEOHAZARDS?

#### PREVIOUS AND ONGOING WORK

Previous and current work is centered on land subsidence, earth fissures, earthquakes, landslides, movement of glaciers and ice sheets. The Arizona Geohazards Research Center (AGRC) was formed in the Department of Civil Engineering & Engineering Mechanics to conduct sponsored, collaborative research and develop technologies to understand, assess and mitigate damages from geohazards.

- > What is the mechanics of the process that causes land subsidence, the formation and growth of earth fissures from groundwater pumping? >How can groundwater resources be managed to mitigate damages to the natural and built environment from land subsidence and earth fissures?
- >How can we model land subsidence and ground fractures in a disordered medium? (Require: multi-physics, multi-scaling approach)
- >How do we design systems to mitigate damages from land subsidence and earth fissures or retrofit existing systems? > What are the potential effects of global climate changes and how to include these effects in managing groundwater resources?





The CAP canal between Shea Blvd Bridge and Via Linda Bridge has subsided differentially by 2 ft. (Photo taken in 2001). Differential subsidence can cause flow reversal, damages to the channel lining and water leaks.

#### Focus Area 2: Landslides, glacier and ice sheets Key issue:

➤ How to predict the movement of landslides, glacier and ice sheets to prevent loss of lives and reduce damages?





The established view has been that large ice masses move slowly and discharge at predictable rates. However, recent data suggests that glacers and ice sheets are inelting more rapidly from global warming and their methods to predict these dimitate change driven movements of glaciers and ice sheets to mitigate damages.

Focus Area 3: Soil liquefaction from earthquakes Key issue:







Flooding in the Happy road area near Phoenix. Flooding caused by land subsidence due to groundwater pumping is a global problem. It

formation and growth of earth fissures and (2) have any good mitigating strategy.

damages to infrastructure and the environment. Extreme climate changes

can lead to increased occurrences of rocksildes due to melting of ice, permafrost thaw and heavier rainfall. A rocksilde in Yosemile National Park in 2008 sent large granile boulders downslope destroying several cabins and injuring three people at a popular lodging area. (Photo: Herb Itum, Associated)

Focus Area 4: Assessment of seismic rockslide

> How to assess the effects of fracture structure on the stability of rock slopes under earthquake loading

vill get worse from global climate changes.

hazard

Key issue:

#### POTENTIAL RESEARCH DIRECTION/PROJECTS

Geohazards are societal problems because they threaten our existence. Our plan is to approach these problems holistically. Thus, we intend to build synergistic research teams that include technical experts, social scientists, policy makers, attorneys, planners, regulators and community leaders. We will expand the current research portfolio to include:

RETENSION SYSTEMS - dams, levees, reservoirs, waterfront facilities and sea defense

LIFELINE SYSTEMS - electric power transmission, water banking, buried pipelines and transportation

EXTREME NATURAL EVENTS AND HUMAN INTERVENTION - debris flow and slope stability, and soil erosion

mining of soil nutrients, urban conversion irrigation, pollution and extreme weather events are increasing soil erosion. Soil erosion (1) damage the environment (2) erosion (1) damage ine environment (2) reduce hydroelectric power production (3) clog rivers, canals and reservoirs with deleterious consequences to agricultural production, water availability, water transportation, fish production, infrastructure and more. This NASA/ISC photo shows erosion of bright-red soils in Betsiboka Estuary, Madagascar.



Debris flows can be catastrophic. They occur suddenly, most often after heavy rainfail, and can deveastate entire towns in minutes. In July, 2006, after 5 days of heavy rainfail, the largest debris flow historically occurred in the Santa Catalina Mountains, Tucson, Arizona. Fortunately, there was no loss of life but considerable damages were done to infrastructure (roads, buildings, hiking trails). Global climate change raise the specter of more frequent and larger debris flow.



Projects will involve developing models, experimental and field verification, risk assessment, mitigation methods, public policy, regulations, codification, integration with geographic information system, instrumentation and monitoring.

#### **KNOWLEDGE/EXPERTISE GAPS**

Geophysicists, groundwater and surface hydrologists, geologists, social scientists, attorneys, planners, policy makers, regulators and

#### **FUNDING OPPORTUNITIES**

Federal: NSF, DOE, NIST, NASA, USDA, FHWA Industry: Water and power providers

State: Legislature, department of transportation, cities, counties and municipalities International: UNESCO, UNDP, etc.

#### Short term funding goal: NSF Geohazards Research Center

Leverage the existing work done by AGRC and expand the research and expertise portfolio to gain funding from NSF to upgrade AGRC to

Long term funding goal: An International Geohazards Research Center

#### PARTICIPANTS (COE AND UA)

COE: Muniram Budhu, Chandra Desai, Lianyang Zhang, Tribikram Kundu, George Frantziskonis, Jennifer Duan, Peter Troch, Juan Valdes



## **Grand Challenges in Resource Development**



## Scope

The advent of the Information Age has demanded an ever-wider range of metallic and non-metallic minerals to perform essential functions. Will the necessary non-fuel mineral resources be available in time and at acceptable costs to meet the burgeoning demand for emerging technologies? The availability of non-fuel minerals and mineral products depends heavily on investments in people and technology. Insufficient investment today will lead to restrictions on availability in the future. ("Minerals, Critical Minerals, and the US Economy", NRC, 2002)



Grand Challenges: Infrastructure, Resources, Energy, Water

### **Questions**

What resources do we have and where?

How do we meet the challenges of sustainable resource development?

How do we lower the spatial footprint of mines?

How do we lower the energy and water consumption used for material production?

How do we minimize environmental disruption?

How do we ensure productive use of land after mining?

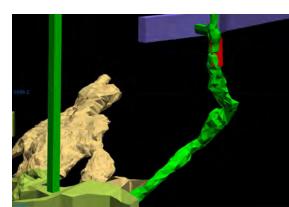
How do we extract resources from deep underground?

How do we extract resources with in situ leaching?

How do we extract resources from the sea and extraterrestrial bodies?

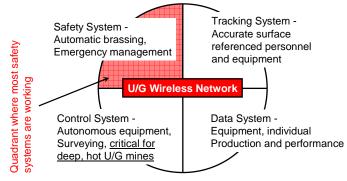


Safety training simulator using software gaming engine from "Real Tournament"



3D laser scan of corkscrew raise from adit to 100-level at San Xavier Mining Laboratory

#### **Vision of the Future of Underground Mining Networks**



Schematic Cross Section of the U/G Network Pipeline

## **Current IMR work**

#### Lower water consumption

•Use of municipal effluent water for flotation

Alternative energy/reduced energy

consumption

- •Solar on mine tailings/mine sites
- •Geothermal
- Changing mining methods to reduce energy consumption
- •Carbon footprint calculations

## Healthy and Safe Communities and

- Community dust exposure from legacy uranium tailings on Navajo Reservation
- •Health effects of biodiesel particulate matter on underground miners
- •Analysis of Australian risk-based approach to mine safety
- Analysis of effectiveness of mine health and safety interventions
- •Miner tracking/communication system
- •Safety training simulator development using gaming engine from "Real Tournament"
  - •Exposure assessment
- •Risk management/intervention effectiveness

#### **Production Technology**

- Equipment automation
- •Mine information technology

#### **Processing Technology**

Improved efficiency of mineral recovery Heavy media separation

#### Fundamental Geosciences

- •Deposit-scale studies focused on adding value in mines and advanced projects
- District to regional scale studies of mineralized regions for exploration, resource assessment, and public policy

#### Economics/Policy

- •Carbon footprint calculations for mine production/processing
- Detailed studies of China and MongoliaCarbon economics
- •Trade-off studies for land use

#### Build laboratory/research capacity

- •Upgrade facilities at the San Xavier Mine
- •Build capacity in mineral processing, geomechanics, and ventilation

#### Build workforce capacity

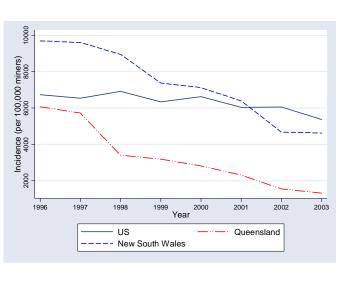
- •Increase graduates, especially future professorate
- •Create 2+2 programs with community colleges



Flotation of chalcopyrite uses 16,800 gal/min of water at one mine



With the atomic force microscope in MGE we can analyze the impact of contaminants in municipal effluent on mineral recovery



The decline in lost time injuries per 100,000 miners was 20%, 78% and 52% in the U.S., Queensland and New South Wales, respectively after Australia adopted a risk-based approach to mine safety.

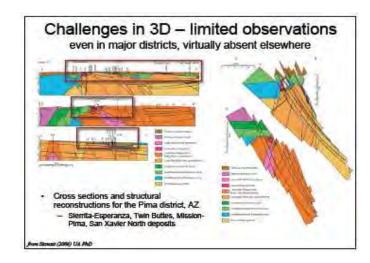


Automation of underground mine equipment – knowing when the bucket is full is a difficult problem.

## **Expertise gaps**

Mine health and safety
Environmental management and mine reclamation
Extractive metallurgy
Mine design

# Why Arizona? World-class mineral endowment - Arizona is the center of one of the world's great mineral provinces - mainly "porphyry copper" but also other kinds of mineral deposits. - Geologically, it contains optimum exposures of the right kinds of rocks - shallow magmatic arc - Few other areas of the world compare - e.g., the central Andes







## **Participants**

Current UA: MGE, GEOS, CoPH Industry: Freeport McMoRan,
Newmont, Resolution Copper,
Peabody Energy, BHPBilliton,
Barrick, AngloAmerican, Caterpillar,
Mineral Zone, Quadra Mining,
Bronco Creek Exploration,
Rosemont Copper, Lowell
Exploration, International Royalty
Corp

**Future:** ENGR, SWES, HWR, AREC, ANTHRO, Eller, Law, Udall, GEOG, SNR, Arid Lands

## Funding opportunities

- •Industry
- •SFAz
- •USGS •NIOSH
- •NSF
- •DOE •EPA
- •Int'l organizations (CRC, AMIRA, etc.)
- NGOs
- •Financial institutions (World Bank, Futures Group, etc.)



School of Sustainable Engineered Systems

## Low ESH-impact Gate Stack Fabrication by Selective Surface Chemistry

New project P10370

Shawn Miller, Fee Li Lie, and Anthony Muscat Department of Chemical and Environmental Engineering University of Arizona, Tucson, AZ 85721





ERC Review Meeting Feb 19-20, 2009 Tucson, AZ Industrial partners:

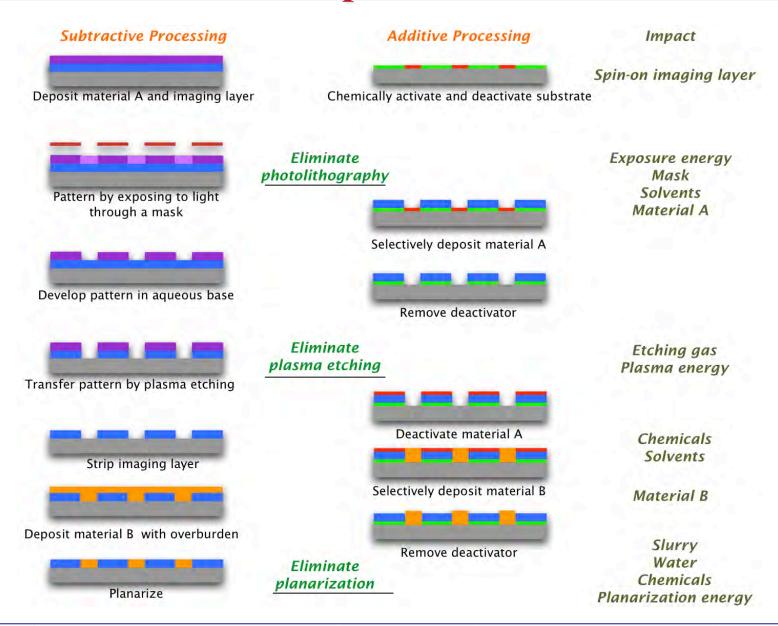
Sematech

ASM, LAM/SEZ

## **Objectives**

- Simplify multistep subtractive processing used in microelectronic device manufacturing
  - Develop new processes that can be integrated into current devices flows
  - Minimize water, energy, chemical, and materials consumption
  - Reduce costs
- Focus on high-k gate stack testbed
  - Fabricate low defect high-k/semiconductor interfaces

## **ESH Metrics and Impact: Additive Processing**



## **ESH Metrics and Impact: Cost Reduction**

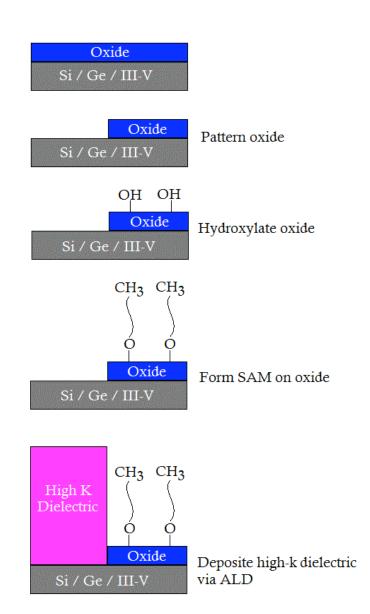
- Integration of selective deposition processes into current front end process flow could reduce ~16% of the processing costs
  - Calculation based on Sematech cost model
  - Eliminate eight processing steps from the gate module
  - Tool depreciation, tool maintenance, direct personnel, indirect personnel, direct space, indirect space, direct material, and indirect material were included
  - Energy, waste disposal, and addition of two selective deposition steps were not included
- There is potential for greater ESH benefit due to minimized cost of raw materials and waste generated

## **Novelty**

- Develop industrially feasible processes to activate and deactivate surfaces
  - Significantly lower time scale
  - Extend to metal and semiconductor surfaces
- Integrate selective deposition steps at carefully chosen points in the CMOS process flow
  - Realize ESH and technical performance gains
- Quantify costs associated with selective deposition steps to refine industry models
  - Account for energy and waste disposal
  - More accurate prediction of the cost model

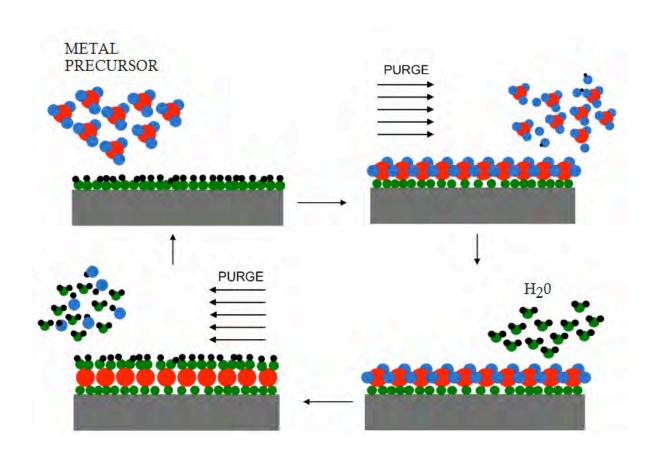
## **Methods and Approach**

- Grow high-k films on semiconductors by activation and deactivation of surface sites
- Activation
  - Utilize surface chemistries to activate substrates for high-k film growth
  - Halogen, amine terminations
- Deactivation
  - Hydrophobic self assembled monolayer (SAM) prevents adsorption of H<sub>2</sub>O
- Model systems
  - Si, Ge, and III-V substrates
  - High-k films
    - Al<sub>2</sub>O<sub>3</sub>
    - TiO<sub>2</sub>
  - Atomic layer deposition (ALD)



## **Atomic layer deposition of high-k films**

- Break overall reaction into two half reactions and run one at a time to achieve self-limiting growth
  - Surfaces exposed to sequential pulses of metal and oxygen precursors to deposit oxide

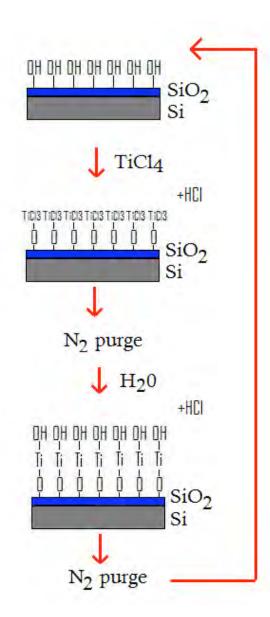


## **ALD Reaction Mechanism**

- Factors governing the selective deposition of high-k film
  - Surface conditioning
  - Precursor selection
  - Deposition conditions
- Hydroxylated surface promotes high-k growth on Si
- Two half reaction in TiO<sub>2</sub> deposition

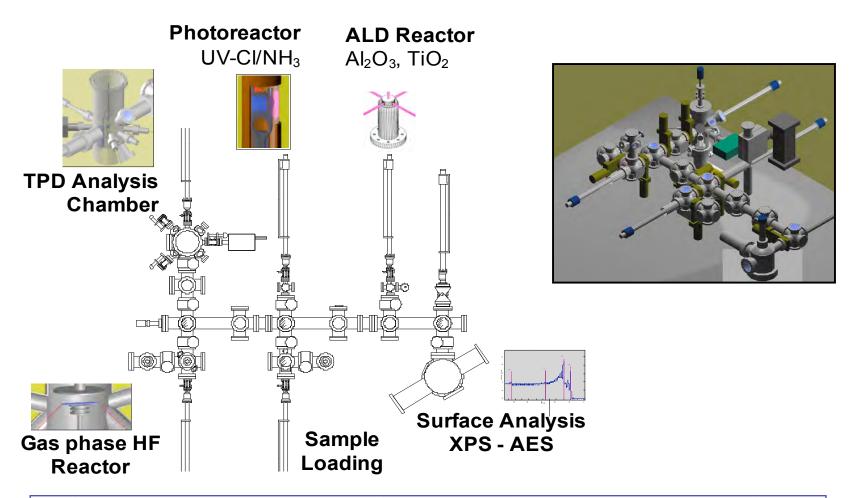
$$TiCl_{4(g)} + -OH \rightarrow -O-TiCl_3 + HCl_{(g)}$$
  
2  $H_2O_{(g)} + -O-TiCl_3 \rightarrow -O-Ti-OH + 3 HCl_{(g)}$ 

 Deposition mechanism using TiCl<sub>4</sub> precursor could be used as a model for HfCl<sub>4</sub> precursor



## **Clustered Research Apparatus**

- In situ cleaning, high-k deposition, and surface analysis enables studies
  of surfaces without atmospheric contamination
  - Important for highly reactive substrate such as III-V materials



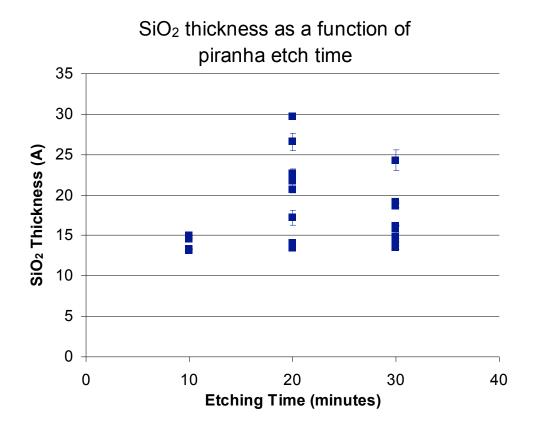
## **Deactivation using SAM Chemicals**

SAM molecules	Formula	Structure
Octadecyltrichlorosilane OTS	C <sub>18</sub> H <sub>37</sub> Cl <sub>3</sub> Si	CI CI CI
Triacontyltrichlorosilane TTS	C <sub>30</sub> H <sub>61</sub> CI <sub>3</sub> Si	CI — Si — CI
Triacontyldimethylchlorosilane TDCS	C <sub>32</sub> H <sub>67</sub> CISi	
Tridecafluoro-1,1,2,2- tetrahydrooctylsilane FOTS	C <sub>8</sub> H <sub>7</sub> F <sub>13</sub> Si	F F F F F F
Octadecyldimethoxysilane ODS	C <sub>21</sub> H <sub>43</sub> O <sub>3</sub> Si	CH3 - 0 - Si CH3 - 0 CH3 - 0 CH3
Trimethylchlorosilane TMCS	C <sub>3</sub> H <sub>9</sub> CISi	CH3     CH3 ~ Si — CI   CH3 /

## Si(100) Surface Preparation: Piranha Etch

#### **Procedure**

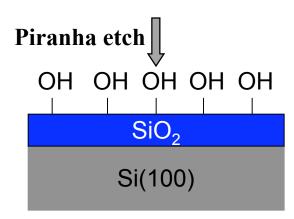
- 5 min sonication in acetone
- 5 min sonication in methanol
- 10 min etch in HF
  - 1:9 HF: H<sub>2</sub>O
- 20 min etch in piranha
  - 110°C ± 10°C
  - -4:1 H<sub>2</sub>SO<sub>4</sub>:H<sub>2</sub>O<sub>2</sub>
- SiO<sub>2</sub> thickness measured with ellipsometer
- 50 ALD cycles of TiO<sub>2</sub>

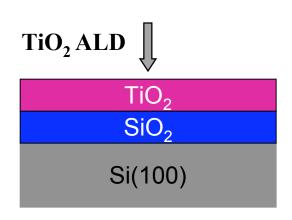


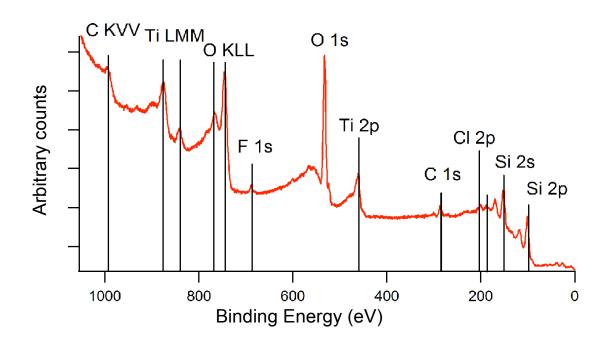
- After piranha etch Si(100) surface was hydroxylated and water contact angle <5°</li>
- Due to scatter of SiO<sub>2</sub> thickness after piranha etch, thickness measurements prior to TiO<sub>2</sub> ALD are necessary

## Si(100) high-k deposition: ALD of TiO<sub>2</sub>





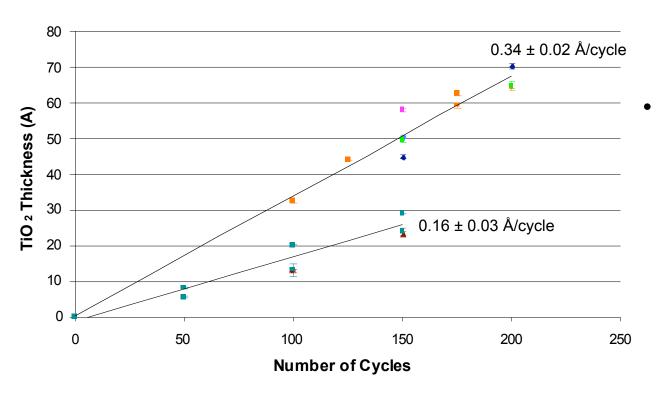


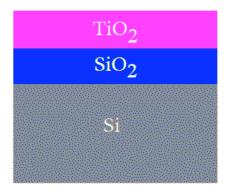


- Demonstrated TiO<sub>2</sub> deposition on hydroxylated Si(100)
  - Residual Cl present on surface
  - Si 2p peak still visible with ~9 Å thick TiO<sub>2</sub>
     layer

## TiO<sub>2</sub> Growth Curve on Hydroxylated Si







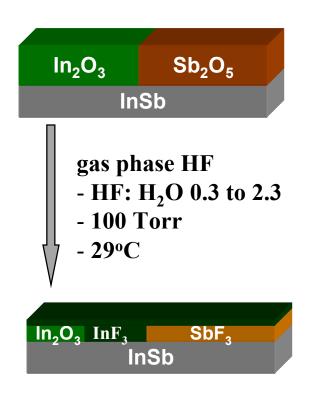
Deposition at 170°C

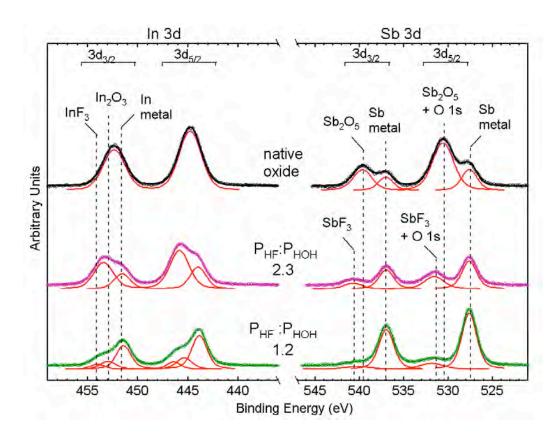
TiCl<sub>4</sub> / Purge / H<sub>2</sub>O / Purge

- 1s / 30s / 0.3s / 60s
- 1s / 30s / 0.3s / 30s
- 1s / 30s / 0.2s / 60s
- 1s / 30s / 0.2s / 30s
- 2s / 30s / 0.2s / 30s
- 2s / 30s / 0.1s / 30s
- 1s / 30s / 0.1s /30s

Optimal deposition parameters:
 1s TiCl<sub>4</sub> pulse / 30s N<sub>2</sub> purge / 0.2s H<sub>2</sub>O pulse / 30s N<sub>2</sub> purge

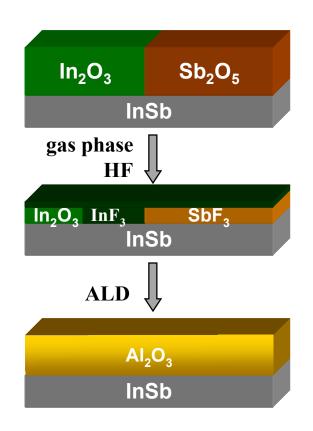
## InSb(100) Surface Preparation: Gas Phase HF

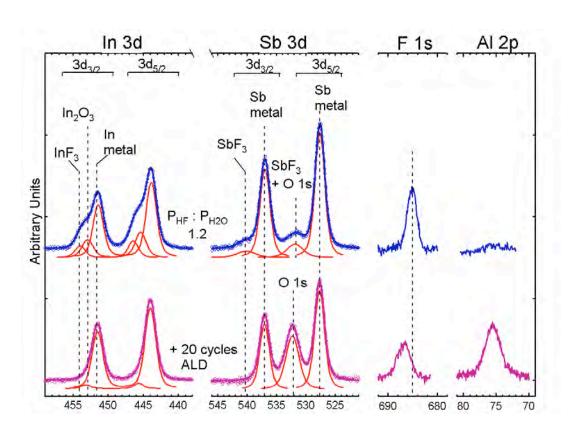




- The nature of defects in III-V native oxide required removing the oxide and replacing it with a high quality dielectric layer
- Oxide removal of InSb(100) native oxide achieved by in situ gas phase HF etching
  - Complete removal of Sb<sub>2</sub>O<sub>5</sub> and partial removal of In<sub>2</sub>O<sub>3</sub>
  - Fluoride surface species consists of SbF<sub>3</sub> and InF<sub>3</sub>

## InSb High-k Deposition: ALD of Al<sub>2</sub>O<sub>3</sub>





- Demonstrate deposition of Al<sub>2</sub>O<sub>3</sub> directly on InSb
  - SbF<sub>3</sub>, In<sub>2</sub>O<sub>3</sub>, InF<sub>3</sub> removed from interface
  - Preferential bonding of O and F to Al
  - In:Sb = 1.2

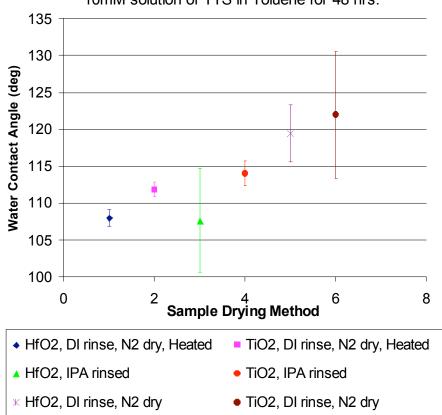
### **Surface Deactivation: SAM formation**

#### **Procedure**

- 5 min sonication in acetone
- 5 min sonication in methanol
- 10 min etch in HF
  - 1:9 HF: H<sub>2</sub>O
- 20 min etch in piranha
  - 110°C ± 10°C
  - 4:1 H<sub>2</sub>SO<sub>4</sub>:H<sub>2</sub>O<sub>2</sub>
- DI water rinsed, N<sub>2</sub> dried
- Remove adsorbed water
  - Heat samples at 200°C, 5 min
- SAM formation
  - 10mM solution of TTS in toluene for 48hrs
- Water contact angle measured

#### **Adsorbed Water Removal**

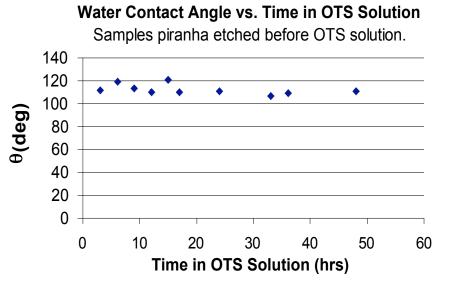
Water Contact Angle vs. Drying Method 10mM solution of TTS in Toluene for 48 hrs.

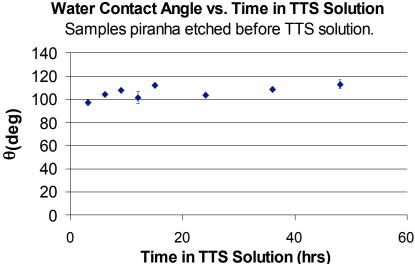


 Polymerization of the SAM molecule was observed due to reaction with adsorbed water producing large deviation in the water contact angle

SRC/Sematech Engineering Research Center for Environmentally Benign Semiconductor Manufacturing

## **Comparison of SAM Molecules: OTS and TTS**





- Similar water contact angle obtained with OTS and TTS
- TTS potentially more effective deactivating agent
  - Higher steric hindrance due to longer carbon chain

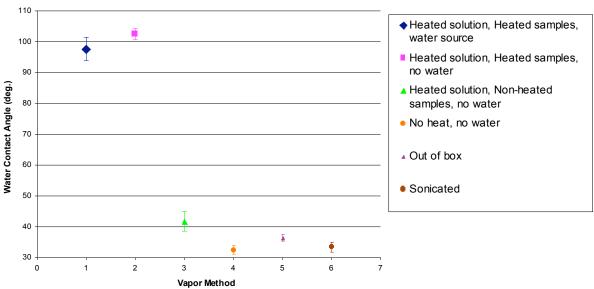
## **Alternative SAM Delivery Method**

- The long time scale for the formation of complete SAM in liquid phase is not feasible for industrial processes
- Vapor phase delivery of SAM potentially shortens time scale

#### Water Contact Angle vs. Vapor Method

Samples piranha etched before vapor being sealed with TTS solution.



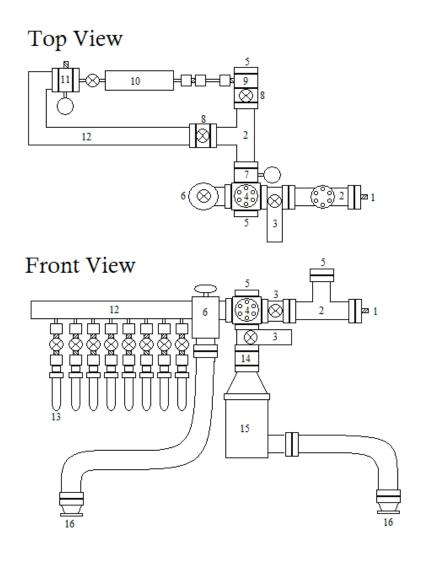


- Demonstrate TTS SAM formation on piranha etched Si(100) by vapor exposure for 48 hours
- Temperature increase required for TTS deposition

### **Future Work**

- Investigate vapor phase ozone and gas phase HF/vapor treatment to increase and control hydroxylation of oxide surfaces
- Characterize SAM layers
  - Thermal stability for deactivation
  - Durability for large numbers of ALD cycles
  - Chemical bonding between SAMs and surface
  - Degradation and repair of SAMs layers
- Extend deactivation study to Al<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, HfO<sub>2</sub> surfaces
- Optimize vapor phase delivery of SAM molecules
  - Pulse and purge both water and SAM molecules as opposed to sealing vapor in a reactor for extended time
- Investigate optimized selective deposition method on III-V semiconductor surfaces

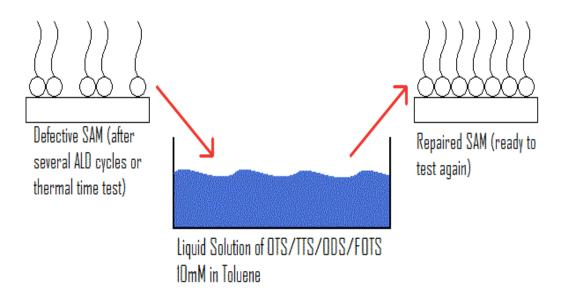
## Future Work: SAM Vapor Phase Reactor Design



- Vacuum vessel designed to optimize vapor phase delivery of SAM molecules
- Delivery cycle consists of alternating pulses of SAM molecules and water with vacuum and N<sub>2</sub> purge between pulses
- Controlled vapor pressure and pulse time capability

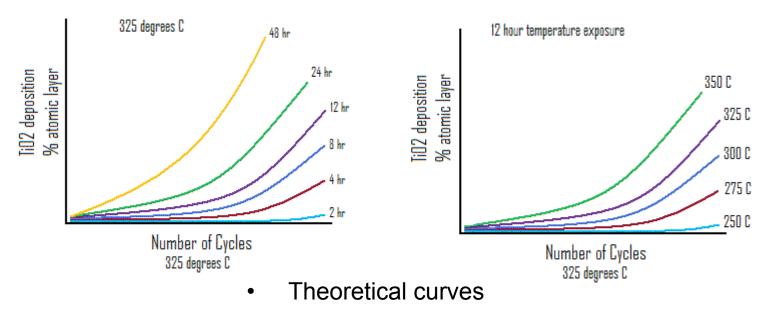
## **Future Work: Repair of SAMs**

- Test restoration/repair of SAMs after maximum # of cycles.
  - Prepare initial SAM using 48 hr liquid submersion
  - Perform maximum number of ALD cycles for which no deposition occurs
  - Repeat liquid coating to reform the SAM layer and repeat all tests
    - Determine maximum number of cycles for the restored SAM using XPS



### Future Work: Thermal Stability of SAM Layers

- Perform thermal time test
  - SAM samples stored between 200°C and 350°C for 2, 4, 8, 12, 24, 48, and 72 hours
  - Deactivation tested for some samples, others will be repaired and tested
    - Test deactivation of ALD for each sample with XPS
  - Determine the maximum # of ALD cycles for which the thermally tested/repaired SAMs are capable of deactivation
    - Compare this to the freshly formed SAMs
    - XPS, FTIR, ellipsometry, and contact angle tests of each SAM



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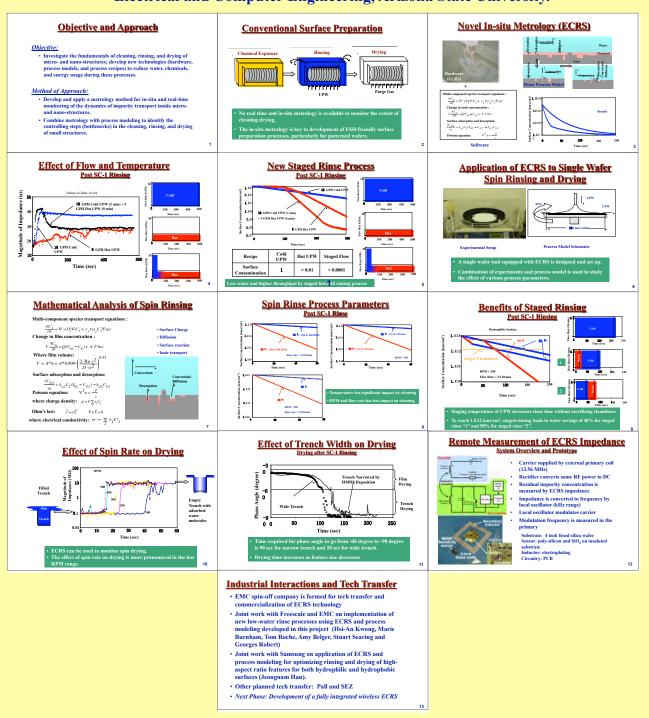
#### **Novel Metrology for Application in Wet Surface Preparation of Patterned Wafers**

Kedar Dhane<sup>1</sup>, Jeongnam Han<sup>2</sup>, Jun Yan<sup>1</sup>, Xu Zhang<sup>3</sup>, Bert Vermeire<sup>3</sup> and Farhang Shadman<sup>1</sup>

Chemical and Environmental Engineering, University of Arizona.

Samsung Electronics Co. Ltd.

<sup>3</sup>Electrical and Computer Engineering, Arizona State University.



# **Energy Saving Opportunities in Mining**



# Scope

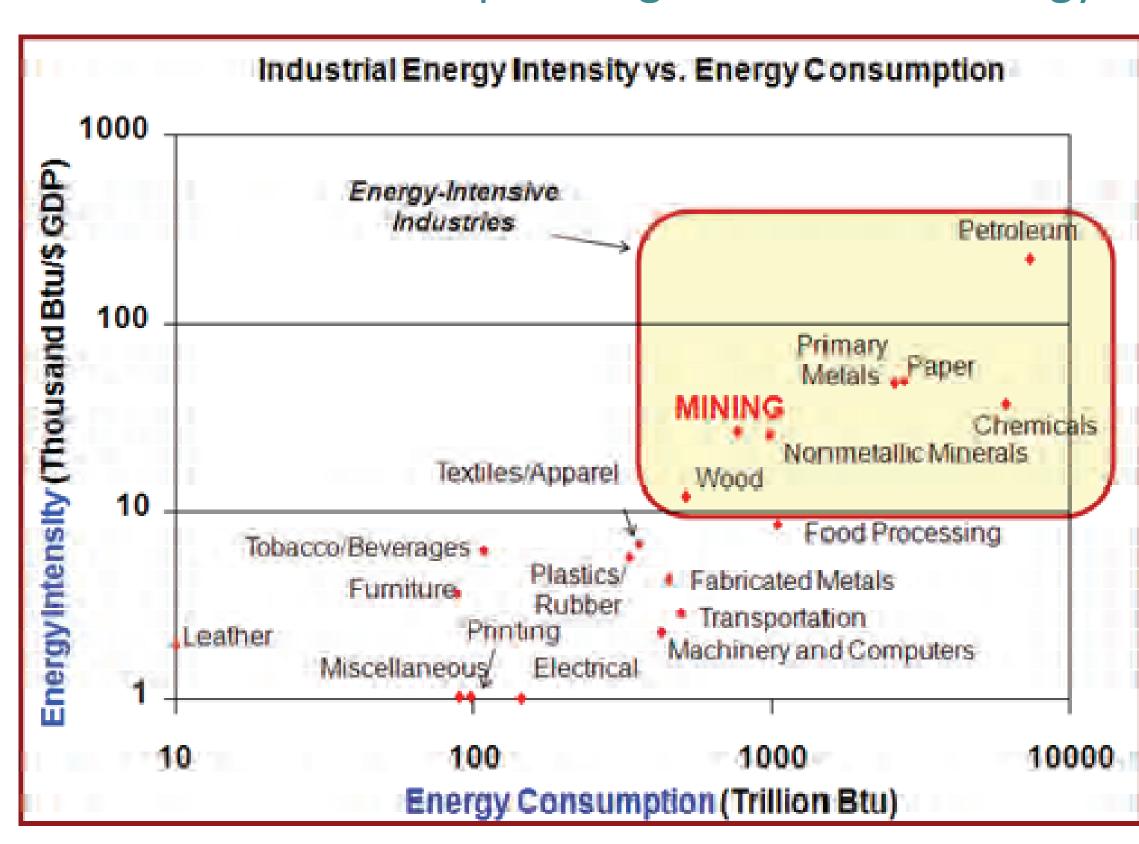
To develop measures, processes and technologies that would reduce the dependency on traditional forms of energy and lower the environmental effect of burning fossil fuels.



Grand Challenges and Theme: Infrastructure, Resources, Energy, and Environment

# Background

 Steps involved in the extraction, processing and transportation of coal, base and precious metals and industrial minerals require large amounts of energy.



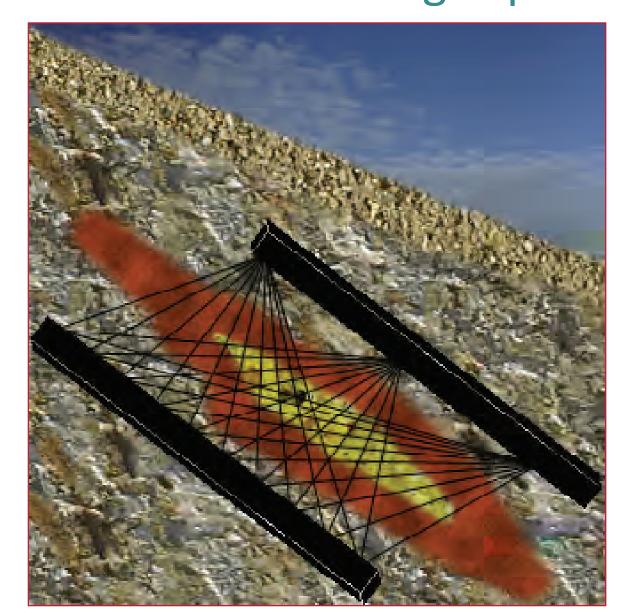
- Cost saving measures can be implemented in two ways: improve the efficiency of processes in order to use less energy, and wherever feasible, substitute the existing supply source with alternative forms of energy.
- Opportunities for energy savings in mining include improving exploration and production techniques such as raising the efficiency of the drilling, excavation, extraction, and ventilation processes; and improving the efficiency of the grinding, crushing, milling, pumping, rolling, and smelting processes.

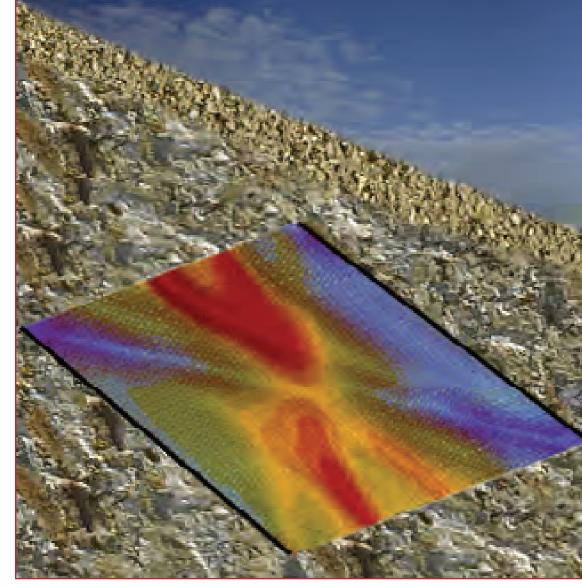
# Previous and Ongoing Work

# Geo-Sensing

 Significant ore reserves are still available for the foreseeable future, however, most reserves are rather concentrated in narrow veins (e.g. inside fault lines) that may or may not be far apart from each other thereby making the task of ore and waste management a vital process in the economic life of the operation.

- Today information regarding the location, shape and size of an ore body is obtained from drilling and recovering core logs which provide a discontinuous and one-dimensional measure of geology.
- Increased orebody sampling in the form of continuous 2D and 3D images (similar to CAT-scan and MRI) made available at a *fraction* of drilling cost would increase the efficiency of cost recovery and minimize environmental disturbances during exploration and mining phases.



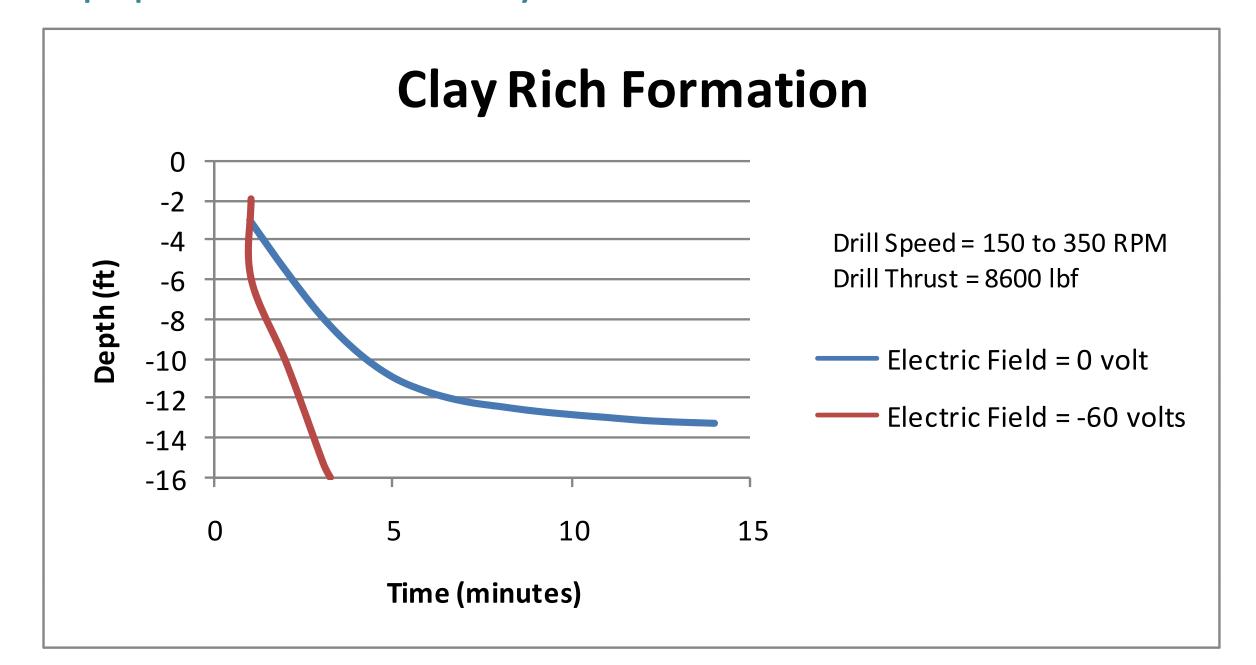


2D Electromagnetic Scan of a Gold Deposit in South Africa

# Rock Softening

- Drilling, sawing and grinding are the most expensive processes in mining as they take up nearly 50% of the total energy consumed by the mining industry.
- Rock breaking technologies are based on one or a combination of the following four components: mechanical fracturing, thermal fracturing, melting, and chemical reactions which require large amounts of energy or are harmful to the environment.
- One phenomenon that has been reported in the literature is the effect of electric currents on the rocks' response to mechanically induced stresses. The underlying mechanism is thought to involve the creation of a layer of negatively charged particles in the vicinity of the rock-tool interface. If this potential is removed, significant increase in the drilling rate along with a reduction in the tool wear can be observed.

 Based on the discovery that stresses applied to rocks activate electronic charge carriers, hence, a current, we propose the reverse of this process: the application of an electric current to alter the mechanical properties of the rocks at the tool/rock interface. Preliminary data confirm the above hypothesis. We are investigating our findings in more detail, since a better understanding of this phenomenon would provide the opportunity to develop more efficient systems that would break rocks faster and require less energy than conventional equipment in use today.



# Low Temperature Geothermal

- The greatest opportunity to utilize geothermal energy in the mining industry is to take advantage of the significant depths to which underground mines are excavated.
- The temperature difference between backfilled spaces and the surface can be beneficially used for heating purposes by installing a closed loop geothermal system.
- Underground water is a valuable source of heat energy (typically between 12°C and 16°C). This heat can be extracted from the water by an open loop system. Our studies have shown that naturally heated water from active or abandoned mines can be used to heat and cool public buildings. Energy savings are estimated to be half-a-million dollars or more.

 We are investigating the possible use of a large mass of broken rock near the surface as a regenerative (periodic or seasonal storage-type) natural heat exchanger. In summer, as the relatively hot intake air flows through the interstices in the broken rock to the ventilation airways, it heats up the rock and, in turn, cools down. In winter, the relatively cold intake air flowing through the broken rock heats up and, in turn, cools down the rock.

# **Potential Research Direction**

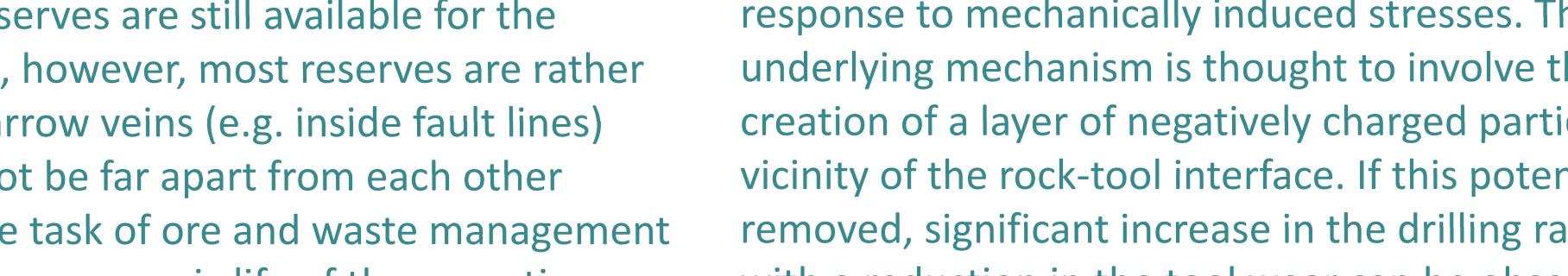
- Develop a 3D rock mass scanner to map fractures
- Develop techniques to estimate ore grade from geosensing data.
- Conduct a fundamental study to determine the underlying driving processes for the rock softening phenomena.
- Develop hybrid systems for drilling and grinding of rocks based on the rock softening phenomena.
- Investigate the use of turbines at the bottom of return pipes in a geothermal system to convert the potential energy of pumped water to electricity.

# Funding opportunities

• Financial support can be sought from NSF, DoE, DoT, SFAz, major mining, petroleum and drilling companies

# Research Partners

- ECE faculty
- MGE faculty
- MSE faculty
- Mining companies
- NASA
- Universities & Research Centers in Canada & Australia





# School of Sustainable Engineered Systems

#### Development of a Center for Multiscale/ Multiphysics Research for Sustainable Engineering Systems

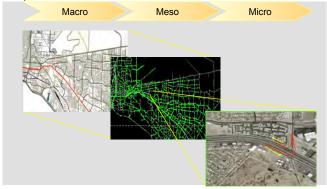
#### Scope

In this poster we propose the development of a research center that will study sustainable engineering systems from a multiscale and multiphysics perspective, combining theory, simulation and experimentation. The center will build on existing expertise on multiscale problems in various areas. Key to the development of the center will be fostering an environment where information and ideas can be shared across disciplines.



#### Issue to be Addressed

Sustainable engineering systems (SES) are complex and multiscale, and mono scale models and experiments are not effective in describing actual SESs. Thus, a multiscale and multiphysics approach to SES holds considerable promise in developing future innovative SESs. Another important question is: for optimal system design which spatial and temporal scales should be resolved?

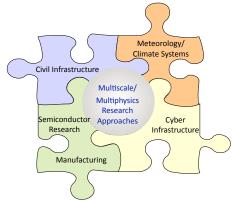


#### **Ongoing Work/ Future Directions**

Since most engineering systems are realization of processes operating over a vast range of length and time scales, various theoretical, computational, and experimental multiscale methods have been developed. Of particular interest to this proposed center are multiresolution methods which can be used for developing multiscale/multiphysics methods. Ongoing multiscale/multiphysics work at UA includes reactive fluid flow, reaction diffusion, chemical reactions, lattice dynamics, material microstructure. Important is the bridging of computational models and simulations to physical experiments performed at various scales. Additionally, areas where engineering systems are studied at various scales include modeling of traffic flow, modeling of climate change, vibration of structural systems.

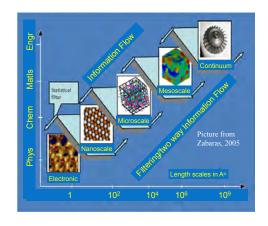
#### **Concept for Development**

The multiscale/multiphysics research approach is cross-cutting that is promising for addressing potentially large-scale and complex engineering problems in various engineering areas. The concepts of the center development starts from forming a group of interested researchers to exchange and share research ideas and modeling techniques, identify external partners, and funding opportunities, with the eventual goal to collaborate in formally establishing a Research Center with external funding.



#### Knowledge/expertise gaps

Even though there is existing expertise in these techniques at UA, it is presently scattered and unorganized, with some researchers unaware of parallel work or application areas where their techniques would have utility. Thus the objective of the center would be to bring together the various researchers in multiscale/ multiphysics techniques to identify and aggressively pursue synergistic work in this area as it applies to sustainable systems, in holding with the objectives of the SSES.



#### **Funding opportunities**

- Infrastructure (NSF, NIST, ADOT, FHWA)
- Energy (DoE, SFAz, NSF, Nat. Labs)
- Environmental/Climate (
- Manufacturing (NSF, DoD, Industry)
- Security (DHS, DoD)

#### **Initial UA/CoE Participants**

Ludwik Adamowicz (Chem)
Yi-Chang Chiu (CEEM)
Pierre Deymier (MSE)
Robert Fleischman (CEEM)
George Frantziskonis (CEEM/MSE)
Krishna Murlidharan (MSE)



SCHOOL OF SUSTAINABLE ENGINEERED SYSTEMS

# Solar energy storage using compressed air in geologic repositories



Laboratory for Advanced Subsurface Imaging (LASI), AzRISE, and Southwest Solar Technologies, Inc.

Research and development on new and improved methods for geophysical surveying of potential salt-cavern compressed-air storage sites

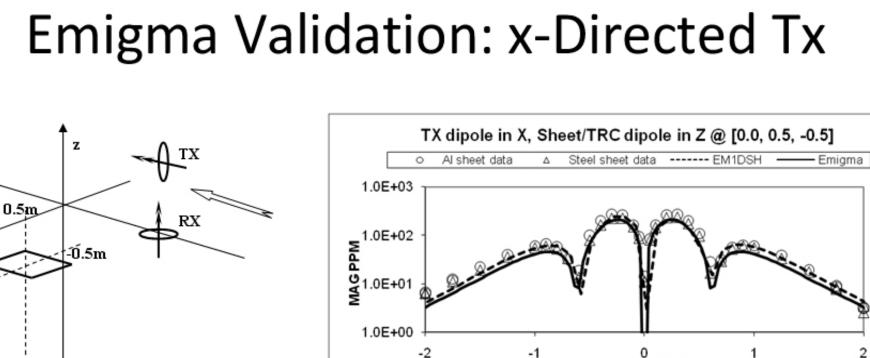
We previously developed a fundamentally new subsurface sensing and imaging method that we call the Alternating Target Antenna Coupling (ATAC) method.

The previous ATAC method is limited to shallow depths, on the order of meters to approximately 10 meters.

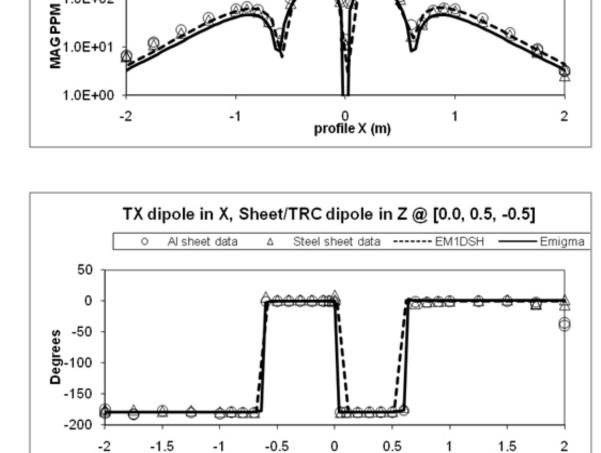
We are currently modifying the ATAC method in order to develop new methods that will lead to revolutionary advances in deep exploration for salt formations.

We plan to use the electromagnetic modeling software Emigma to test our new high-sensitivity array.

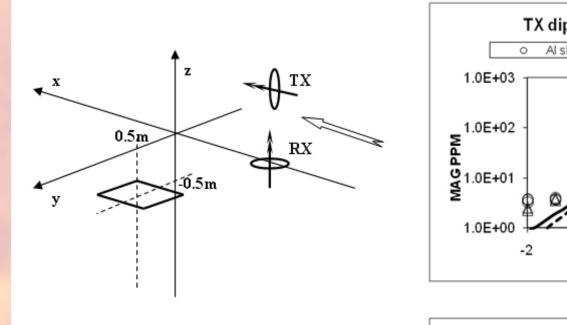
However, first we validated Emigma by using one of our previous test geometries.



 The plotted data are for a survey carried out along the x axis using the ATAC method. The Emigma results are in excellent agreement with the measured results and the



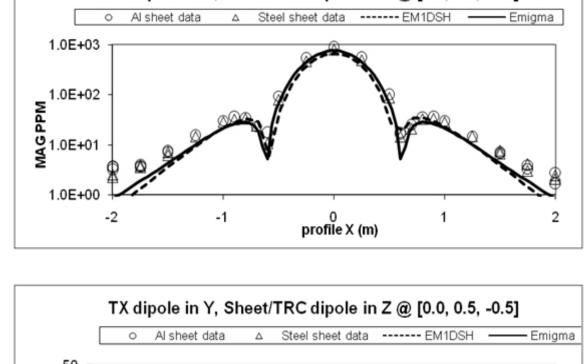
# Emigma Validation: y-Directed Tx

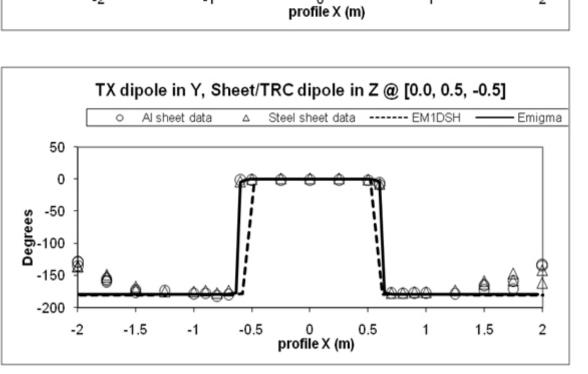


 Now the Tx is rotated to the The plotted data are for a survey carried out along the xaxis using the ATAC method. The Emigma results are once again in excellent agreemer

with the measured results and

the EM1DSH results

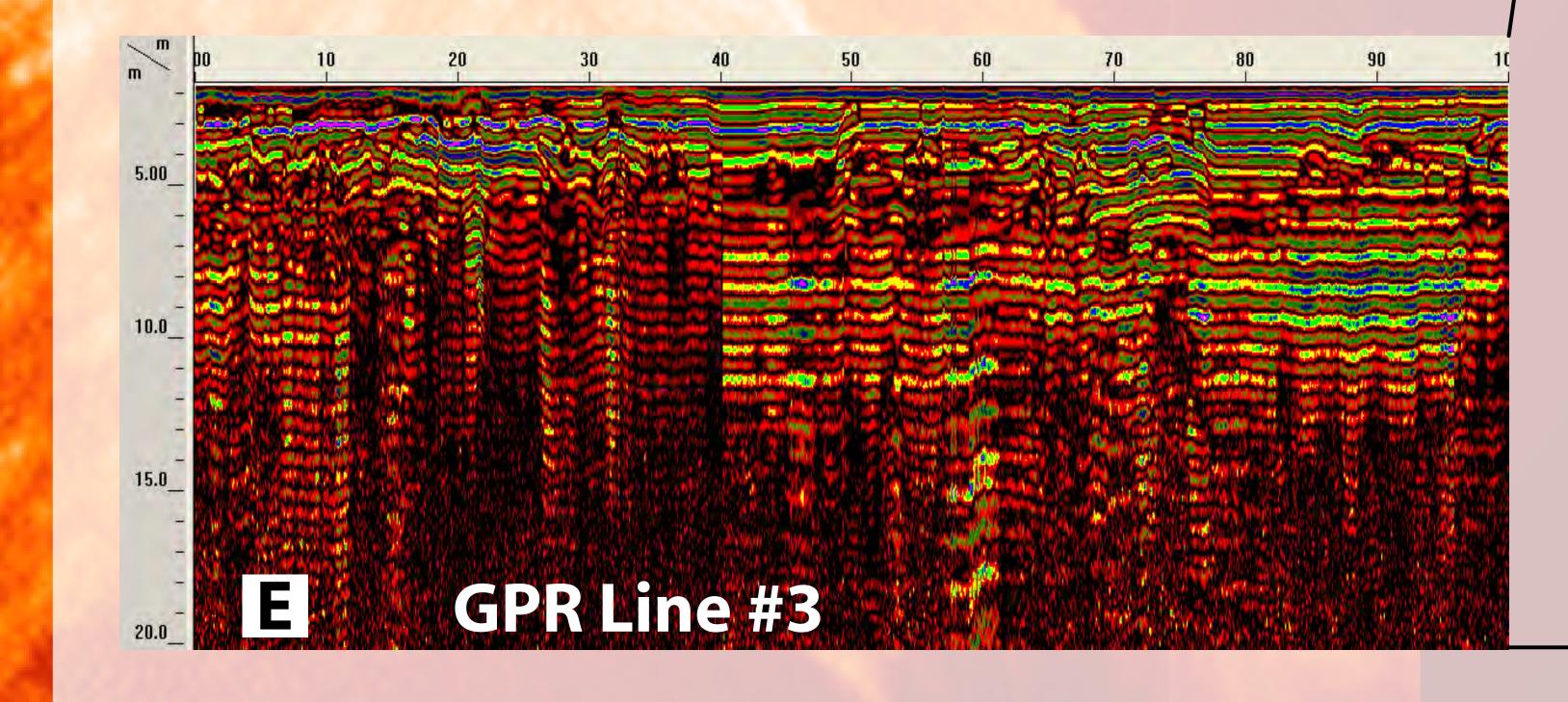




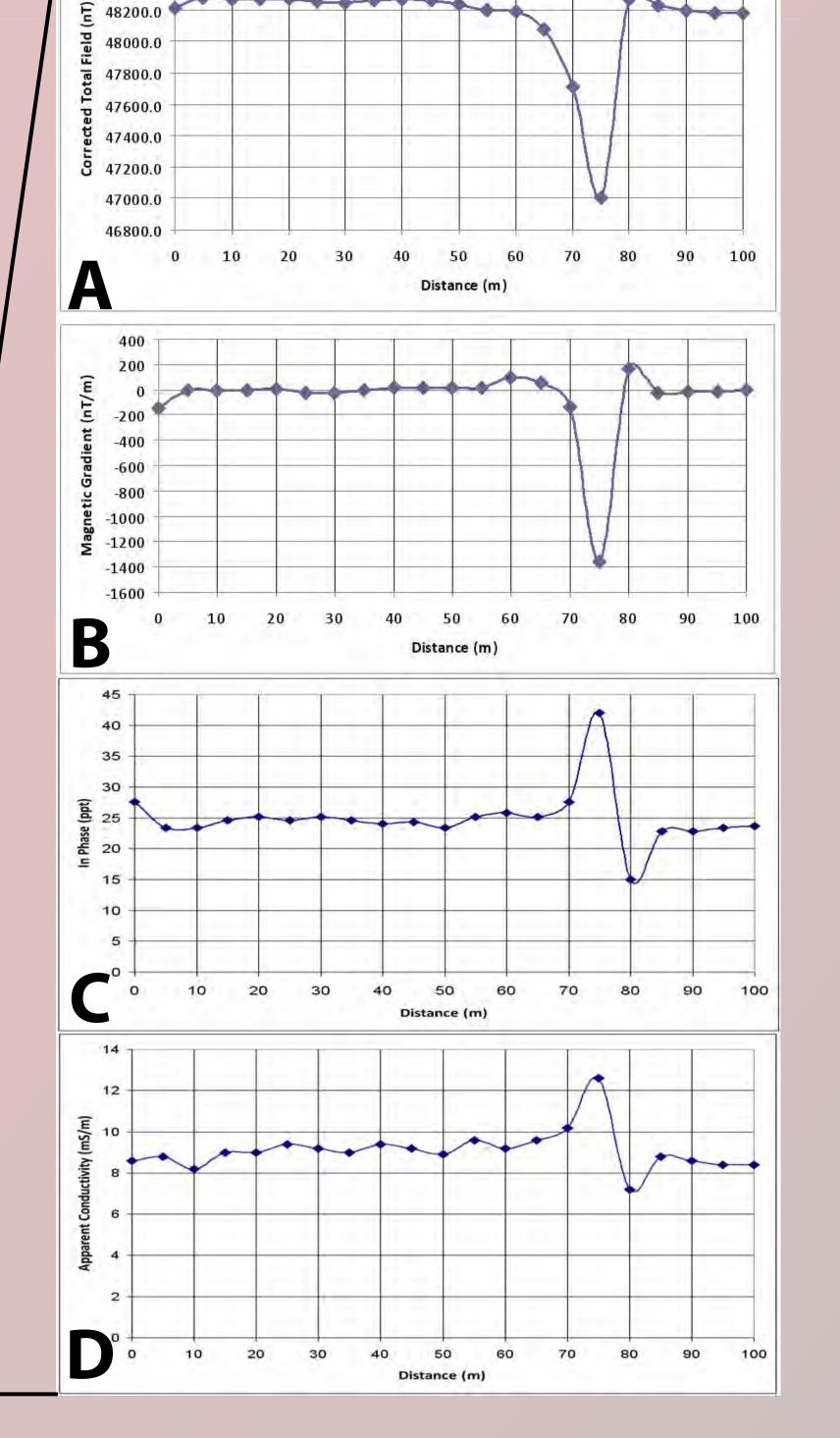
Geophysical investigations of potential sites for compressed air storage facilities



Numerous geophysical techniques were used at the planned Riverpoint Solar Research Park to help characterize the site's potential for underground compressed air storage. Site-wide measurements included: A: Total magnetic field; B: Magnetic gradient; C: In-phase ratio of secondary to primary magnetic fields; D: Apparent conductivity; and E: GPR analysis of subsurface features. Results indicated some areas with large, buried metallic objects that should be avoided.



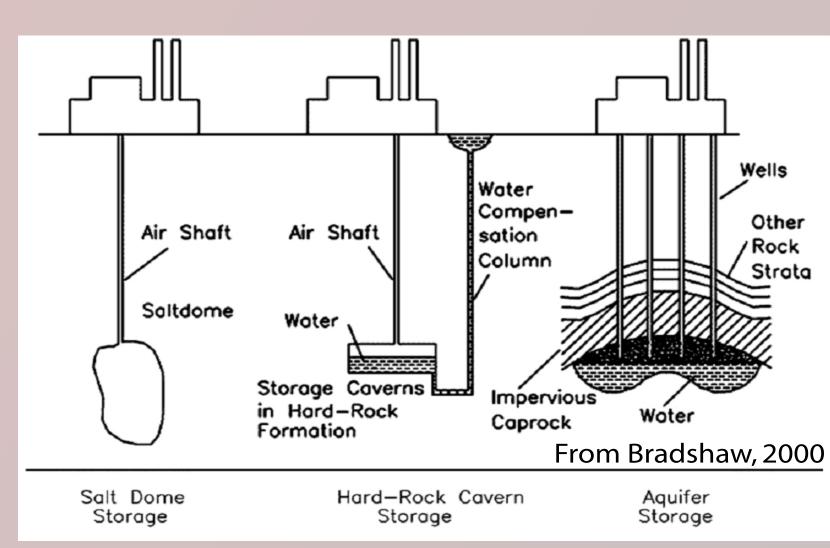




# Geotechnical safety of potential methods for storage in geologic repositories

Compressed air energy storage (CAES) in the subsurface is a promising method for storing solar energy.

This project studies the geotechnical safety of potential methods for storing compressed air in shallow alluvium.

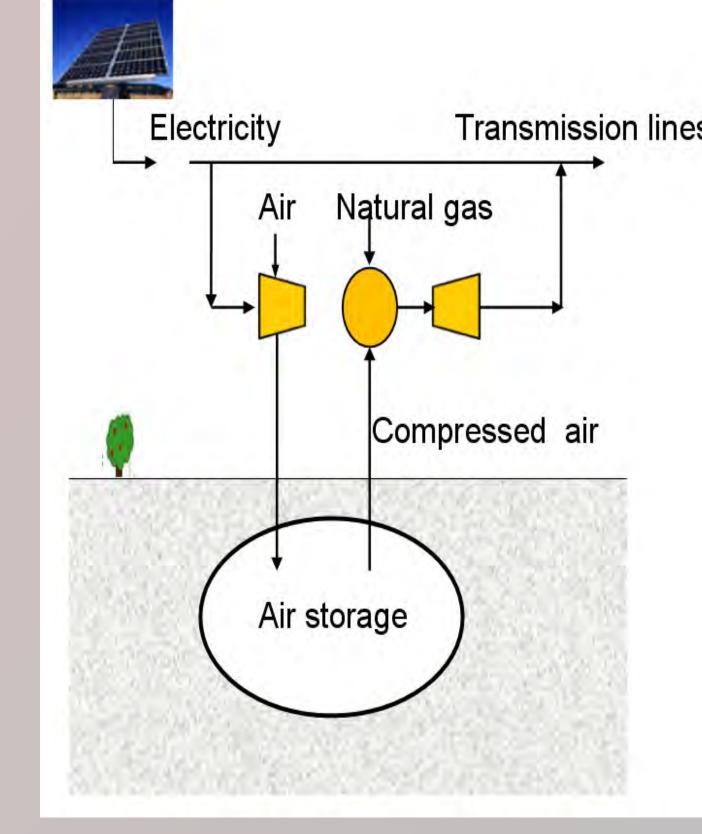


# Large-scale methods:

- -Solution mined salt caverns
- -Hard rock caverns
- -Aquifers or abandoned mines

# **Small-scale methods:**

- -Steel tanks
- -Pipelines



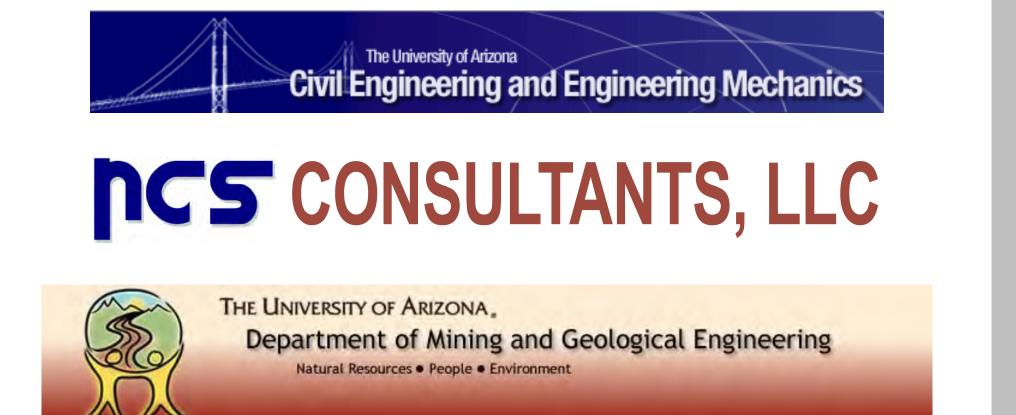
# **Major Issues:**

-Air tightness -Stability of surrounding soil mass (consider high pressure and daily loading-unloading

# **Solutions:**

-We are in the process of developing new techniques for the safe and efficient underground storage of compressed air.







# Ben Sternberg Phil Stokes

Laboratory for Advanced Subsurface Imaging UA Dept. of Mining & Geological Engineering

# Lianyang Zhang Saeed Ahmari

Dept. of Civil Engineering University of Arizona

# Steve Dvorak

Dept. of Electrical Engineering

University of Arizona

# Dept. of Materials Science Engineering University of Arizona

Joseph Simmons

# Herb Hayden Sonya Dancoe

# Southwest Solar Technologies, Inc Phoenix, AZ

# Ed Nowatzki, Randy Post & Naresh Samtani

# NCS Consultants, LLC Tucson, AZ

# Shoba Maraj, Nick Barbato & Sarah Grubaugh

#### Winning the Global Race for Solar Silicon



#### Scope

A new refining process, utilizing an oxi-nitride slag, under investigation for producing low cost solar Si has the potential to reduce the cost of Si used in photovoltaics by 50%. Refining of silicon is the most expensive step in producing a photovoltaic panel, amounting to 25% of the final cost. Cost reductions all along the value chain, and new developments in concentrators, will make electricity generated from polycrystalline Si solar cells competitive with fossil fuels produced electricity.

Grand Challenge: Energy & Environment - Making Solar Energy Economical



#### Technical Objective

- Reduce B and P content in Si to 1 ppmw or lower
- Design, build, & operate modular production unit for solar silicon
- Continue to improve refining process
- Explore other optional routes for producing low cost solar silicon
- Overall goal is to establish Arizona as the number 1 producer of solar silicon.

#### **Benefits for UA & Arizona**

- Education center Emphasis on processing materials for PV
- Establish Tucson as the nation's center for purification and processing of materials for PVs
- · Generate permanent jobs
- Creation of new wealth for the UA and the people of Arizona

#### **Previous and Ongoing Work**

- IP disclosure, Sept. 2002
- · Experiments run at NTNU, 2004
- · Dow Corning tests in Brazil, 2005
- STRC formed, Nov. 2006
- STRC & UA sign license agreement, Sept. 2007
- US patent application published Oct. 25, 2007
- International patents applied for Sept. 2008
- World-class melting facility up and running since mid Dec., 2008
- Initial testing has yielded phosphorus reduction from 35 to 3 ppmw and boron reduction from 20 to 8 ppmw, objective is 1 ppmw each at a slag to Si mass ratio of 0.2



UA & STRC Melting Lab

#### **Potential Research Direction/Projects**

- Continue development of UA/STRC refining process.
- Develop modified Silgrain Process (acid treatment of silicides for impurity removal with additional emphasis on P).
- · Design & development of modular production unit.
- Explore potential of wafer back-grinding slimes as feed material for UA/STRC refining process
- Continue to work with NZ companies to commercialize process for utilizing local high purity quartz sands for production of silicon as feed material to the UA/STRC refining process.

#### **Knowledge/Expertise Gaps**

- We are working in a chemical system for which there is very little thermo-chemical information. Fundamental investigations of the thermodynamics, viscosity, and density of the slags are critical to understanding the refining process.
- Fundamentals of the kinetics of the transfer of B and P to the oxi-nitride slag need to be investigated.
- Development of economical process for producing nitrides.
- Commercialization of the process will require developing new refractory materials that resist chemical attack by both molten silicon and the oxi-nitride slag.
- Thermodynamic calculations reveal that solid oxi-nitride phases have significantly greater potential for refining of molten silicon, and could lead to simpler continuous processing. Such solid-liquid processing poses additional problems, including kinetics and transport issues, structural strength, and solid particle sintering.
- Development of a modified Silgrain process for acid treatment of silicon for impurity removal.
- Dewatering and beneficiation of wafer back-grinding slimes represents a significant source of relatively pure silicon as feed material.
- Processing of high purity NZ quartz sands for reduction in a modified silicon submerged arc furnace.

#### **Research Team and Associates**

• Working with 9 Companies, 1 National Lab & 3 Other Universities (Located in 7 States, and 6 Other Countries)



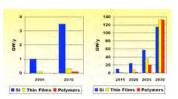
- Faculty & Technicians Involved at UA
   Professor David Lynch (thermo-chemical processing)
   Professor Jinhong Zhang (beneficiation & dewatering)
   Tim Corley (chemical analysis)
- Would like to involve faculty with expertise in: Hydrometallurgy (possibly Professor Hiskey) Ceramics

Induction heating (currently working with Ajax-Tocco) Microwave heating

Mine survey (possibly UA's MGE Department) Economic Evaluation (possibly Professor Arnold)

#### **Funding Opportunities**

- Funding to date more than \$1.5 million (\$1.2 million from industry).
  Notified last week that SBIR Phase I Proposal
- to NSF is approved for funding.
- Additional funding during the research stage can be sought from NSF, DoE, SFAz, and industry.
- Funding for commercialization of process can be sought from industry, investors, NY State Economic Development Council, and NZ Federal Government



Source: EPIA / RWE Schott Solar (2004)

Although the role of Si in PVs is expected to decline, it is still expected to be a growth industry for the next 20 years.

#### **UA/STRC** vs Competitors

Our competitors using metallurgical refining techniques have difficulty in removing P from silicon, with reported distribution ratios of P in slag versus that in SI of only 0.1 to 0.3. In the few months we have been running experiments we have achieved distribution ratios for P of 1.4 to 29. The UA/STRC process has a distinct advantage in removing phosphorus from silicon.



**School of Sustainable Engineered Systems** 

#### Scaled Demonstrator of Solar Tower Plant

#### **Hermann F Fasel and Andreas Gross**

#### Scope

We propose to employ commercial fluid dynamics and structural analysis software for designing a solar tower plant with 44m tower height that will allow for scaled investigations of the characteristics of MW-class full size plants. The proposed demonstrator will be instrumented for scientific analysis and also permit studies of the environmental properties and agricultural potential of the collector greenhouse

Federal funding is mainly being channeled into photovoltaic (PV) research and development. Simpler and more robust technologies such as solar tower plants attract little support. Our proposed research will proof that solar tower plants can be a viable alternative to PV arrays.

Areas of Challenge Theme are Resources, Energy, and Environment

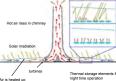


Prototype of solar undraft tower in Manzanares, Spain

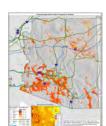




### Operating principle







Large areas with less than 1%

The Southwest has

for solar power

tremendous potential

power output is directly related to collector size,  $A_{coll}$  and tower height, h,



 $g=9.81m/s^2$ ,  $c_p=1005.b!(kgK)$ ,  $T_0$  is ambient air temperature, and G=1  $m^2$  is solar irradiation ollector efficiency, η<sub>c</sub>=0.8 and η<sub>col</sub>=0.6



Solar tower plants are scalable:



#### Focus of proposed research

- In the US focus has been on solar trough and PV technology for solar power
- Currently available photovoltaic (PV) power conversion units are not competitive when compared with conventional power plants in terms of cent/kWh (the unit production cost is very high and system performance typically degrades considerably over life span)
- · Solar-thermal power conversion technologies, such as the solar tower concept, promise to be more cost effective for large power plants than PV systems
- · Solar tower plants do not require high-tech production facilities and can be operated and maintained by relatively untrained personnel
- · Solar tower plant technology is investigated in Europe and Australia but not in the US · Solar tower plants are ideally suited for Arizona and the Southwest of the US
- · Proposed research program will
- > allow the country to catch up with competition from abroad
- benefit the nation and Arizona as it will provide a solar power generation alternative that is both, inexpensive and low maintenance
- · If technology can be brought to full scale application it will provide jobs and considerably cut back on greenhouse gas emissions and reduce dependence on fossil

#### Knowledge/expertise gaps

- · Solar tower plants have the potential to provide a lost-cost and low-tech alternative to PV based solar power generation. Issues related to the fluid- and thermodynamics of the collector and the structural design of the tower have to be addressed to provide the confidence level necessary for the construction of MW-class plants.
- · In addition, the collector area can potentially be used for greenhouse farming which may create jobs in agriculture. Research regarding the environmental conditions under the collector is needed to determine the agriculture suitability for more arid climates such as Southern Arizona.

#### Previous work

- · We designed and built a scaled demonstrator of the Manzanares power plant for laboratory experiments
- The demonstrator is equipped with instrumentation for obtaining temperature and velocity measurements
- · We also carried out a preliminary computational fluid dynamics (CFD) analysis of the 3x3ft solar tower laboratory model



#### **Proposed research**

- We propose to employ Computational Fluid Dynamics (CFD) and structural analysis software (FEM) for designing solar tower plants with tower heights of up to 100m that will allow for scaled investigations of the characteristics of up to 200 MW full size plants.
- · Explore novel ideas for substantially decreasing the tower height (tower constitutes major cost of plant)
- The proposed demonstrator will be instrumented for scientific analysis and also permit studies of the environmental conditions under the collector. This will determine the agricultural potential of the collector greenhouse.

We propose to build several solar tower demonstrator plants with scientific instrumentation

Power output [kW]	Tower height [m]	Collector (greenhouse) diameter [m]	Collector area [m²]	Tower diameter [m]
0.1	19.8	24.8	483	1
1	42.8	53.5	2,250	2.2
10	92.2	115.3	10,400	4.7
100	198.6	248.2	48 400	10.2

We have established a business contact with Schlaich Bergermann Solar GmbH, Stuttgart, Germany who designed and and built the solar tower prototype plant in Spain.

#### **Funding opportunities**

The proposed work has high potential for obtaining funding from DOE or NSF and industry

#### **Participants**

The main part of the proposed research will be carried out by researchers at the Aerospace and Mechanical Engineering Department at the University of Arizona. The proposed research will also include researchers from the College of Engineering and the College of Agriculture and Life Sciences.

The PI has close contact with R. Bergermann who was the program manager for the solar tower prototype in Manzanares, Spain, who is currently co-owner of Schlaich Bergermann Solar. The PI has written confirmation that Schlaich Bergermann Solar is willing to cooperate with him on this project.

Hermann F Fasel Aerospace and Mechanical Engineering Department University of Arizona Tucson, AZ 85721 (520) 621-2771 faselh@email.arizona.edu

Andreas Gross agross@email.arizona.edu



#### **Sustainable Manufacturing in Supercritical Carbon Dioxide**

#### Scope

Abstract text in 28 pt Arial

This is the right

Include Grand Challenges and Theme (Infrastructure, Resources, Energy, and **Environment)** Limit to this area This is the right



#### Central issues to be addressed

- Reduce environmental burden of manufacturing
- · non-toxic solvents
- · recyclable processing methods
- Improve manufacturing technology
- · new nanomaterials with novel behavior
- · higher extraction efficiencies

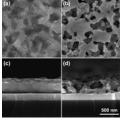
#### Previous and ongoing work

#### **Nanostructured Materials**

#### Synthesis of nanoporous Ag by dealloying

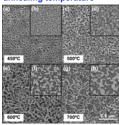
- · Cu is selectively etched from within a AgCu alloy
- · Removal occurs by selective oxidation and chelation
- · Nanoporous structure can be tuned by processing conditions

#### SEM images before and after dealloying



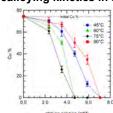
FESEM images of AgCu films topdown (a) alloyed (b) dealloyed and cross-sectional (c) alloyed (d)

#### Increased feature size with annealing temperature



FESEM images of AgCu samples alloye (inset) and dealloyed with increasing anneal temperature (a) and (b) 450°C, (c)

#### Dealloying kinetics in supercritical CO<sub>2</sub>



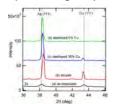
Remaining Cu composition as a function of etching solution concentration at temperature of 45, 60, 75, and 90°C, 0.55 g/cm<sup>3</sup> scCO<sub>2</sub>

Remaining Cu composition as a function of H<sub>2</sub>O<sub>2</sub>/hfacH molar ratio at 60°C, 145 bar, and 3 min reaction time.

### Potential research direction/projects

- · Nanoporous Ag for chemical/biological sensors
- INSERT SENSOR SCHEMATIC
- · Catalytic properties of nanoporous Ag
- · Synthesis of soft, heat-sensitive nanomaterials
- polymer composites
- · metal-organic framework (MOF) materials
- ADD DIRECTIONS FOR ALGAE PROJECT

#### Nanoporous Ag Properties



XRD spectra for AgCu films (a) as-deposited (3x) (b) alloyed at 450°C for 2.5 hours (c) dealloyed to 35\% Cu (d) dealloyed to 0\% Cu.

IIV-vis absorbance spectra of nnAg from in situ and stepwise-dealloyed AgCu compared to an

#### Knowledge/expertise gaps

- · Surface chemistry of inorganic solids in supercritical CO<sub>2</sub>
- Structure-property relationships
- Laboratory to industrial scale-up
- Optimized conditions for desired product outcomes

#### Oil Extraction from Algae

- · Dissolve oil in pressurized supercritical CO,
- Recycle/reuse CO<sub>2</sub>
- Improved extraction efficiency
- · Compatible with wet and dry algae feeds
- · Benchmark against conventional two-stage cold press system



- **Funding opportunities** National Science Foundation (NSF)
- Department of Energy (DOE)
- United States Department of Agriculture (USDA)

#### Participants (COE and UA)

- College of Agriculture
- Biochemistry

azengineering

SCHOOL OF SUSTAINABLE **ENGINEERED SYSTEMS** 

## Sustainable Resource Development **Of Critical Earth Materials**



### Scope

Obtaining a social license to operate means making mineral resource development compatible with local community interests and environmental protection while balancing the need for a reliable global supply of materials.





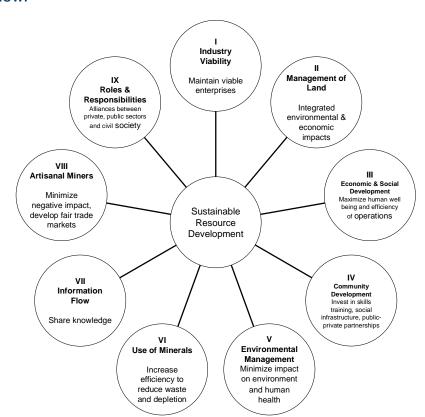
### **Definition**

"Sustainable development is one of a range of ideas about how humans should best interact with each other and the biosphere. The Rio Conference in 1992 established three pillars of sustainable development: economic, environmental, and social

At the heart of sustainable development are the five main forms of capital

- •Natural capital: a continuing income from ecosystem benefits including mineral resources
- •Manufactured capital: infrastructure
- •Human capital: knowledge, skills, health, culture
- Social capital: structures that allow groups to develop collaboratively
- •Financial capital: value of which is representative of other forms of

Sustainable **resource** development provides a framework for the minerals sector as a whole to contribute to human welfare and wellbeing today without reducing the potential for future generations to do the same." ("Breaking New Ground": MMSD, 2002). The Nine key challenges of sustainable resource development in the minerals sector are shown below.



The nine key challenges of sustainable resource development as defined in the Mining, Minerals, and Sustainable Development report "Breaking New Ground" (MMSD, 2002).

The long-term goal of the Institute for Mineral Resources (IMR) is to be able to address all of the nine key challenges of sustainable resource development



### Context

The University of Arizona is one of very few institutions in the world with the depth and breadth to lead research in sustainable mineral resource development (University of British Columbia and University of Queensland are other strong schools). We have the only university in the world with mining engineering, geosciences, and public health programs collaborating. The addition of world-class expertise in hydrology, environmental science, resource economics, applied anthropology, policy, and law gives the UA Lowell Institute for Mineral Resources unique strength to tackle the difficult challenges of sustainable resource development on a global basis.

### **Previous work**

- •Occupational safety and health of miners and mining communities in sub-Saharan Africa (MGE, CoPH, NIH Fogarty International Center Grant, WHO, Int'l Labor Organization on Occupational Safety and Health in Africa)
- •5 in-country epidemiological studies in Zambia
- •1 in-country short course in Zambia
- •The Mitigation of Environmental Disturbances in Ecologically Sensitive Habitats by Artisan and Small-Scale Miners in Developing Regions of the Guyana Shield (MGE, CoPH, Industry, US State Department, Conservation International)
- •Technical assessment of the Marcopper Mine disaster in Marinduque, Philippines (MGE, Futures Group, USGS, Army Institute for Pathology)
- •UN Conference on Trade and Development assistance to government of Mauritania on innovative policies (MGE,
- Probabilistic Approach to Project-Specific Political Risk Analysis for Mineral Projects (MGE, Barrick)
- •Comparison of risk-based and compliance-based safety management systems (MGE, CoPH, NIOSH)

### Potential research direction/projects

- •Life cycle analysis and footprint calculations for material consumption
- Materials flow analysis
- Recycling (e.g. e-waste)
- Ecosystem modeling
- Community social responsibility
- Community health
- Economic trade-off analysis
- •Clean water for communities
- Artisanal small scale mining and poverty alleviation
- •Indigenous peoples
- Land use planning
- Mineral laws and policy
- Large-volume waste handling
- Mine closure planning
- Management of metals in the environment
- Management of biological diversity
- •Environmental management systems



### Future: ENGR, SWES, HWR, AREC, ANTHRO, Eller, Law, Udall, GEOG, ATMO, SNR, Arid Lands

## **Expertise gaps**

Current: MGE, GEOS, CoPH

•Mine environmental management and reclamation tied to mine design

**Participants (COE and UA)** 

- Mining sustainability
- Recycling

## **Funding opportunities**

- •USGS
- NIOSH
- •NSF •DOE
- •EPA
- Int'l organizations (UN, CRC, AMIRA, etc.)
- •NGOs
- •Financial institutions (World Bank, Futures Group,



School of Sustainable **Engineered Systems** 

#### Flow Control for Wind Turbine Applications

Andreas Gross and Hermann F Fasel

#### We propose to employ Computational Fluid Dynamics (CFD), wind tunnel experiments, and a model wind turbine for investigating passive and Active Flow Control (AFC) concepts for wind turbines. Flow control will permit wind turbines to start at lower wind speeds. Active Flow Control (AFC) will also allow for a fast, efficient, and localized response to wind gusts and wind speed fluctuations. The proposed research will improve the efficiency of existing wind turbine designs and may lead to new more light

Areas of Challenge Theme are Resources, Energy, and Environment





The US Department of Energy's (DOE) National Renewable Energy Laboratory (NREL) 10-meter diameter research wind turbine which was tested in NASA's 24.4 by 36.6 meter (80' by 120') wind tunnel.

#### Focus of proposed research

- Pitch control systems can lower the required starting wind speed and increase performance. These systems, however, add complexity to an otherwise simple system. · Modern large wind turbines are subject to significant unsteady loads resulting from wind shear, gusts, large scale atmospheric turbulence, yaw misalignment, upwind wakes, and aeroelastic vibration of the blades
- · Wind gusts (sudden change in wind speed and/or direction) can quickly drive the turbine operating state out of the nominal region and into rotational augmentation or dynamic stall which are characterized by large unsteady aerodynamic loads and acoustic noise.
- The operating limitations imposed by static and dynamic stall as well as rotational augmentation can likely be overcome using passive and Active Flow Control (AFC) devices without the need for a major redesign. Active Flow Control in particular could also reduce noise and fatigue loads which would allow for more light weight designs.
- Design is always a compromise and pitch control can only account for gradual variations in the wind speed. We believe that Active Flow Control (AFC) is a suitable and economically viable method for responding in the required timely manner and in a distributed fashion to the unsteady and local variations in wind speed.

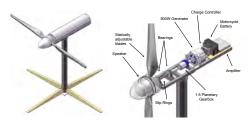
#### **Knowledge/expertise gaps**

- · In the past, company emphasis has been mainly on the development of larger wind turbines where the design was mostly conventional and the technology was based on earlier research and development. Aerodynamic efficiency and acoustic noise seem to haven taken a backseat compared to other components, which were deemed more important, such as gearbox, generator, structural design of the blades, and controller design. For example, currently used wind turbine airfoils date back to the 1990s Clearly, a renewed and substantial effort has to be made to focus on aerodynamics and aero-acoustics of wind turbines
- · A multitude of aerospace applications have shown that aerodynamics performance can be increased significantly with passive and Active Flow Control (AFC). Although efforts are being made to transfer flow control technology to wind turbine applications significant breakthroughs have not been accomplished.

#### NRFL S809 airfoil



#### Our 1/5 scale model of the NREL turbine:



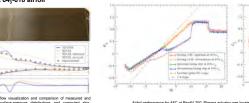


#### Previous work

Scope

- · We have extensive experience with active flow control (AFC) for low-pressure turbines (LPTs) and uninhabited aerial vehicles (UAVs). In particular, we have employed Computational Fluid Dynamics (CFD) and wind tunnel experiments for investigating passive and active flow control strategies (pulsed vortex generator jets and plasma actuators) for controlling laminar separation for LPT blades and UAV
- · The simulations allowed us to extract the relevant physical mechanisms responsible for the stunning effectiveness of pulsed VGJs. We found that by far the most effective and efficient flow control is obtained when inherent flow instabilities are exploited. The CFD results were validated in the wind tunnel
- · We designed a 1/5 scale model of the NREL 10m wind turbine which is equipped with pulsed vortex generator jets. The model is currently being built and will be tested.
- . The NREL 10m wind turbine S809 airfoil is being tested in the wind tunnel. This allows us to determine optimal operating parameters

#### NACA 64<sub>2</sub>-618 airfoil







#### Proposed research

- · We propose to employ Computational Fluid Dynamics (CFD) and wind tunnel experiments for investigating passive and Active Flow Control (AFC) strategies for wind turbine applications. Active flow control strategies will include fluidic actuators (pulsed vortex generator jets and bi-stable "flip-flop" jets) as well as plasma actuators.
- The detailed and highly resolved flow data obtained from CFD simulations will allow us to extract the relevant flow physics. A well founded understanding of the physics will greatly enhance chances for a successful and effective wind turbine flow control
- Wind tunnel experiments will be carried out to validate the CFD results and quickly scan large parameter spaces.
- · Flow control strategies that are deemed successful will (if possible) be tested on our 1/5 scale model of the NREL 10m wind turbine. These tests will pave the way for a transfer of technology to full size wind turbines

#### Funding opportunities

The proposed work has high potential for obtaining funding from DOE or NSF and industry

#### **Participants**

The main part of the proposed research will be carried out by researchers at the Aerospace and Mechanical Engineering Department at the University of Arizona.



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Hermann F Fasel faselh@email.arizona.edu



## **Optimization of Water Resources**



## Scope

The coupling of artificial neural networks and non-linear optimization allows better predictive capability for natural systems and when combined with non-linear multiobjective optimization we can manage resources to accommodate conflicting objectives in real time.



Grand Challenges: Water – better real-time management tools

### Issue

The science of hydrogeology has devoted significant effort and resources to understanding and modeling the movement of groundwater through subsurface systems. Over the last hundred years or so, great advances have been made, from Darcy's formulation of his porous media flow law to the development of advanced numerical flow models. Still, it is widely recognized that our ability to accurately simulate groundwater flow with numerical models is inherently limited by simplifying model assumptions (e.g., laminar flow) and parameter uncertainty (e.g., hydraulic conductivity). Artificial neural networks (ANNs) offer a powerful alternative for modeling and predicting groundwater responses.

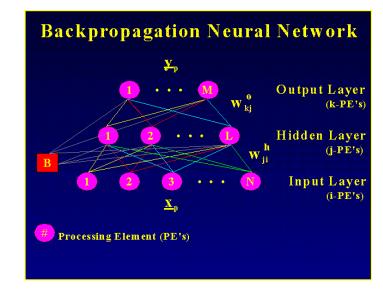
### **Background**

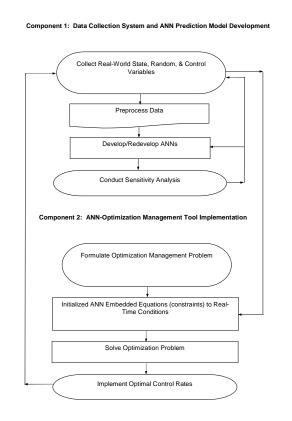
Researchers at the University of Arizona were the first to propose using ANNs for predicting transient head values in real-world groundwater systems in response to both weather and pumping conditions. Unlike a physically based numerical flow model (such as MODFLOW), an ANN does not require explicit input of hydrogeologic parameters and boundary conditions, such as hydraulic conductivity, aquifer thickness, storativity, or recharge rates. Instead, the ANN requires historical data on head values, pumping rates, and weather conditions. By processing this data, the ANN "learns" how water levels at measurement points of interest respond to variable pumping and weather conditions.

In several case studies ANNs have achieved superior head predictive capability, even outperforming extensively calibrated numerical flow models.

US Patent 7254564 Technology Transfer:







Potential research direction/projects

•Inclusion of geostatistical variations in aquifer properties

•Application to manufacturing facilities

Adjustment to physical changes in system

Application to mines

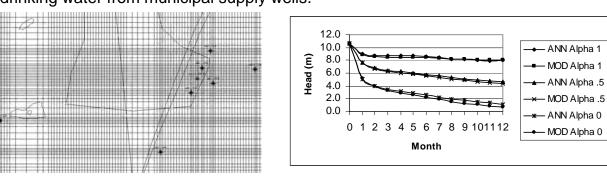
Error calibration

Time sensitivity

### **Previous work**

#### Managing Contaminant Plume/Maximize Fresh Water Supply

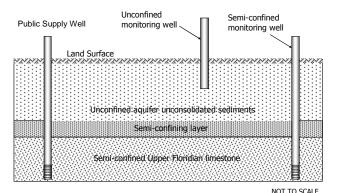
A ten million dollar epidemiological study conducted over six years in Toms River, NJ, found a statistically significant correlation between incidence of leukemia in young girls and exposure to contaminated drinking water from municipal supply wells.

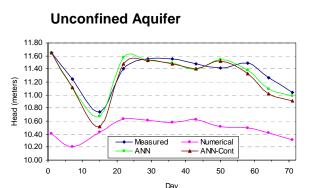


NJ State Hydrogeologist concluded that ANN results provided higher measure of safety and more defensible than policy derived with MODFLOW trial and

error. ANN Method State Trial and Error W22 = 337 gpm.W22 = 600 gpm.W24 = 700 gpm.W24 = 600 gpm.W29 < 200 gpm. W29 = 0 gpm.W44 = 450 gpm.W44 = 513 gpm.

#### Minimize water level decrease in wetlands

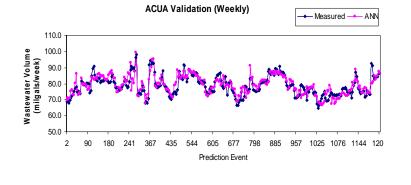




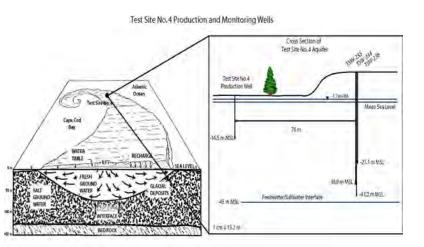
#### Forecast wastewater volume for Atlantic City

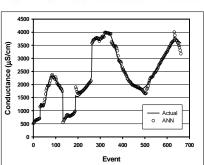
Forecast wastewater volumes for the next day, the next 7-days, and the next 30-days.

Wastewater volume predicted on the basis of three variable types; lagged wastewater volumes, lagged weather conditions, and "future" weather conditions.



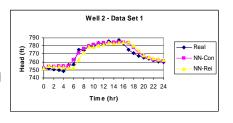
#### Salt-Water Upconing Prediction Provincetown, MA





#### **Minimize Energy for Pumping**

Find the most efficient way of using 11 high-capacity wells in Eden Praire, MN, to minimize the energy cost of pumping the wells.



### **Participants (COE and UA)**

Current: MGE. SIE. HWR

Mary Poulton, Ferenc Szidarovszky, Emery Coppola,

### **Funding opportunities**

NSF

•DOE

•EPA

Industry

# azengineering

#### Scope

A novel type of a Vertical Axis Wind Turbine that accounts for all the shortcomings of is predecessors was designed (See Fig. 8). It relies heavily on the use of Active Flow Control. A two pronged approach is suggested: (1) Investigate fundamental issues of separation control and flow induced oscillations on this design. (2) Build a "proof of concept" comparative model and test it in the field.



# DESIGN & BUILD A VERTICAL AXIS TURBINE THAT OVERCOMES THE PREDECESSORS' SHORTCOMINGS

- Use Active Flow Control (AFC) to provide the starting torque needed to initiate rotation and increase the operational envelope of the turbine
- •Use sweeping jet actuators (Fig. 3) that have no moving parts but need some compressed air to start operation and to increase operational envelope of the turbine (Fig. 4).
- •Delay the onset of dynamic stall by using AFC (Fig. 5), providing a different turbine shape (Fig. 8) and by employing novel airfoil sections (Fig. 6)
- •Eliminate the central tower by using different support system, thus reducing substantially the wake-rotor blade interaction (Fig. 8).
- •Stop AFC when the wind exceeds the design speed limit. This will automatically stall the rotor blades decelerating them rapidly (self feathering). Design features listed below stem from the fact that a turbine is embedded in earth's boundary layer & the loads on it are horizontal (Fig. 7)
- •Change the shape of the classical Darrieus Turbine (Fig. 1) by eliminating its converging top that stalls first.
- Change the guy wire supports to relieve the pressure on the bottom bearing.
  Use an open truss to reduce the drag on the horizontal strut
- •Make the height of the bottom strut adjustable to conform with the wind velocity profile on the selected site.

THESE FEATURES ARE REPRESENTED IN FIGURE 8

#### Potential research direction/projects

- Build a wind tunnel model to test the novel concepts and assess the significance of wind speed on the power generated by the new turbine
- Build comparative wind turbine demonstrators using a STEM senior course in the Nogales AZ. School System and the Academy for Math & Physics.
- 3. Use CFD for predictive purposes and optimization
- Increase the scale fro 10ft to 100ft height in cooperation with DOE
- Consider various means of storage and transmission
- . Put forth a business model aimed at reducing the cost per KWH

#### **Funding opportunities**

DOE, DOD or DOT for special applications NSF, sustainability office for identifying and solving fundamental design issues.

#### **UA Participants**

AME,SIE, ECE
Business school at the U of A
The Bellows Foundation

# Fig. 3 Sweeping jet actuators

Fig. 4 Improvement of airfoil characteristics

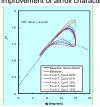


Fig. 5 The use of AFC to delay dynamic stall

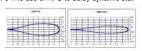


Fig. 6 Replace the NACA0015 airfoils used by Liebeck's symmetrical airfoils





Fig. 7 Wind profile and typical loads on a Darieus turbine

### COMMON, HORIZONTAL AXIS WIND TURBINE HAS THESE SHORTCOMINGS

- Requires large foundation
- Requires a rigid tower and & rotor
- Costly to transport & maintain because machinery and generator are on top
- . Noisy and inappropriate for floating offshore operation
- · Has to be aligned relative to the wind
- Has a complex pitch control mechanism

#### VERTICAL AXIS WIND TURBINE

#### Pros

- Omni directional (Fig. 1)
- •Simple rotor blade that is uniform along the span
- •Machinery and generator are on the ground
- •Requires a small foundation and is amenable to offshore operation thus reducing environmental impact
- •Amenable to active flow separation control

#### Cons

- •Provides a low torque at start and may require external starter (Fig. 1)
- •Experiences dynamic stall somewhere along its span, particularly on its upper part
- •Guy wires anchoring the turbine load the bottom bearing
- •Horizontal braces cause large losses due to their drag

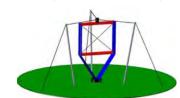


Fig. 8 Schematic design of a novel vertical axis turbine

U.S. Provisional Patent Application filed.



Fig. 1 The Classical Darieus Wind Turbine installed by Hydro Quebec, CANADA

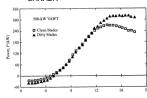


Fig. 2 Power vs. wind speed m/s

