



Prezentarea rezultatelor științifice în SESIUNE DE POSTERE

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Facultatea de Chimie Industrială și Ingineria Mediului**

Synthesis of Cubic Au Nanoparticle Supports for Trichloroethene Remediation

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2. Motivation

- Understanding Structure: To better understand the effect of Au's crystalline structure on the catalytic mechanism
- Improvement: To improve the reaction rate

3. Cubic Au Nanoparticles

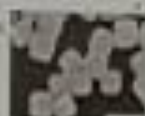


Spherical NPs surface are composed of many crystallographic facets

- Important consideration for catalysis
 - 111 facet only visible surface
 - Type of crystalline facets may affect rate

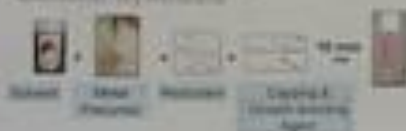


- Others have developed cubic Au NPs
 - Many (111) facets exposed



- Replace spherical NPs with cubic ones

General Synthesis



4. Directed-Growth Mechanism



Surface-selective capping agent controls growth and crystal facets

- Proposed Shape Development**
- Applied to Au, Pt, or even Ag
 - The kinetic energy can help this mechanism

5. Cubic Au Nanoparticle Syntheses & Results

Method	Gold Precursor	Reducing Agent	Capping Agent	Temp.	Yield
Seed Growth	AuCl ₃	Hydroxylamine	PVP	100°C	100%
Reduction	AuCl ₃	Hydroxylamine	PVP	100°C	100%
Reduction	AuCl ₃	Hydroxylamine	PVP	100°C	100%



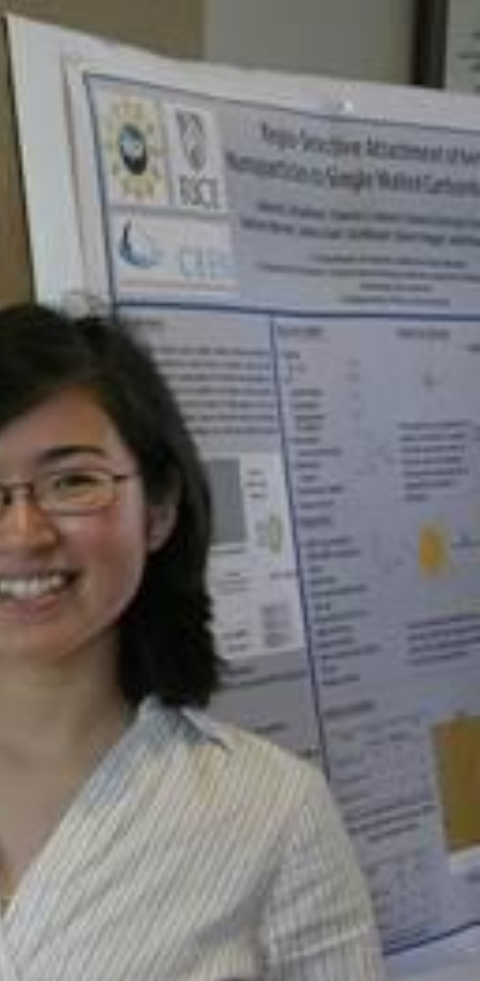
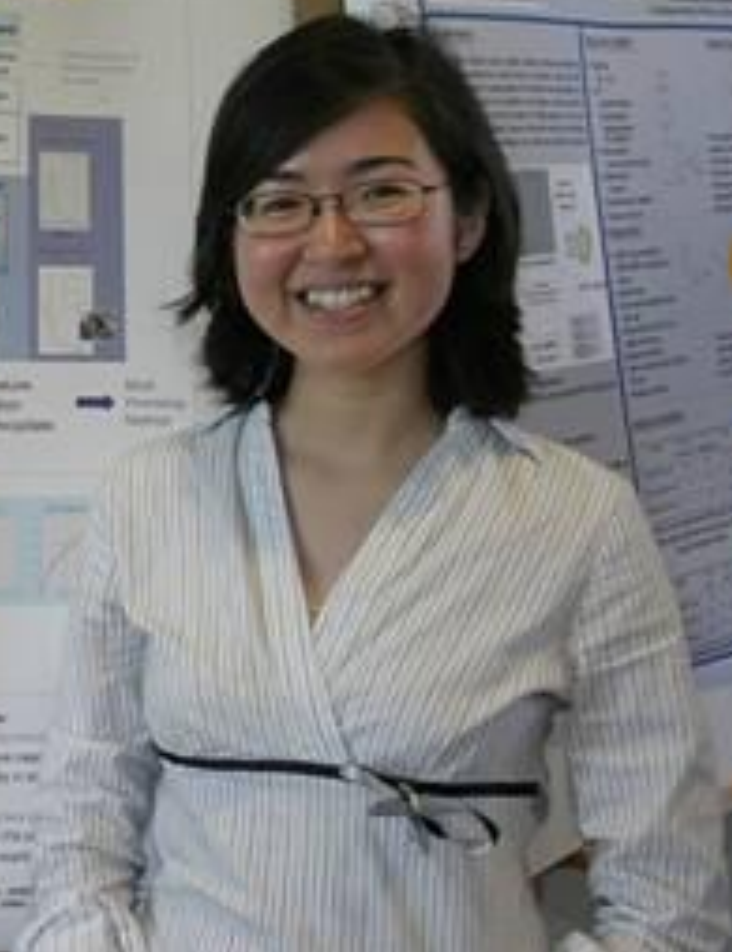
- Features:
 - Controlled Size
 - High Yield
 - High Purity
- Advantages:
 - Increasing surface area
 - Facilitates catalysis
 - Difficult to reproduce
- Disadvantages:
 - Higher temperature
 - Aggregation tendency
 - NPs do not precipitate

6. Discussion

- Hydroxylamine (Ox) method for Au NPs synthesis
- Why?**
- Controlled size to precisely 111 surface exposure
 - High yield, without phase transfer
 - Low concentration of water

7. Conclusions

- Plan
 - Developed synthesis route for Au NPs
 - Controlled surface area (111)
 - Observed effect on catalysis rate
 - Observed high catalysis with seed method (Au, Ag, Pt) at 100°C
 - Surface area of high temperature
- Future efforts
 - Controlled size
 - Controlled shape
 - Controlled yield
 - Controlled purity
 - Controlled stability
 - Controlled reproducibility
 - Controlled cost
 - Controlled toxicity
 - Controlled environmental impact



Nuclear Nonproliferation Initiative Strategic Plan

VISION: to be a recognized technical and program leader providing nuclear nonproliferation services to the nation. In so doing, the Laboratory will support the nation's goals for global security and stability, and will further international acceptance of advanced nuclear energy systems.

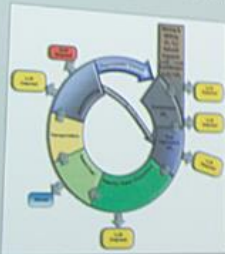


Step 1 of a Strategic Plan is to create and set out a Vision of the ideal future and what the company wants to strive for. The Nuclear Nonproliferation Initiative (NNI) Vision above is an example.

Step 2 is to survey the market "landscape". The table above is an element of the nonproliferation "landscape". The three regimes of Nonproliferation in the table are part of a synopsis of the nonproliferation sector. An outline of the sector in broad market details gives a general framework to explain the limitations of the Plan, then follows a detailed analysis considering the limitations of competitors. This includes a breakdown of the customers' needs and spending habits. For instance, the pie graph on the right explains the Nonproliferation Budget for DOE. Next competitors' capabilities, financial resources, and critical infrastructure are assessed. Examples from the NNI Plan are pictured on the right and include a visual illustrating the competitors' areas of specialization and a percentage pie graph showing market share.



Step 3 is to conduct an **organizational assessment**. This includes an evaluation of the business's personnel, infrastructure, financial status, and market infiltration. For example, during our assessment INL's involvement in nearly all the fuel cycle steps pictured below was taken into account.



Step 4 is to identify **Objectives**, outline **Strategies**, and develop **Plans** to implement these strategies in order to accomplish the Vision while considering the business vision, market landscape, and organization assessment. The NNI Objectives are below.

OBJECTIVES: to identify shortfalls within the current nuclear nonproliferation market; to build a solid and recognized base of sustainable research and business; to enhance complementary research; and to promote, develop and maintain relationships

Visualizing Sensitive Oxidative DNA Lesions

Main Oxidative DNA Lesions 8-oxodG
 dG Exhibit Strongly Different Pairing Properties



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Introduction

DNA due to oxidation is believed to be a major cause for the development of cancer and the process of aging. The formamidopyrimidine derivatives 8-oxodG (β-8-oxodG) and 7,8-dihydro-8-oxodG (β-FaPydG) are the two main oxidative DNA lesions induced by oxidative stress. As a monomeric nucleotide, β-FaPydG readily anomerizes in solution, improving its incorporation into oligonucleotides by a machine assisted DNA synthesis.

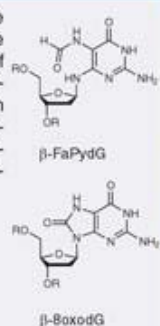
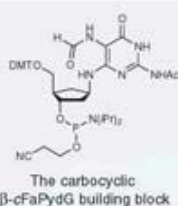


Figure 1: Anomerization equilibrium of FaPydG.

Goals

Develop a β-FaPydG building block suitable for automated DNA synthesis. The carbocyclic analog β-cFaPydG (β-cFaPydG) fulfills these requirements.



Incorporate β-cFaPydG into oligonucleotides for automated DNA synthesis.

Compare the UV-melting points of DNA duplexes containing β-cFaPydG. Compare with the melting behavior of duplexes containing 8-oxodG and unmodified dG.

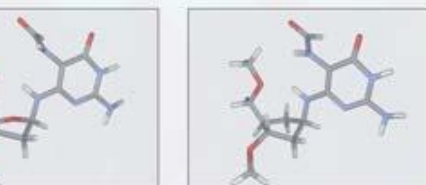


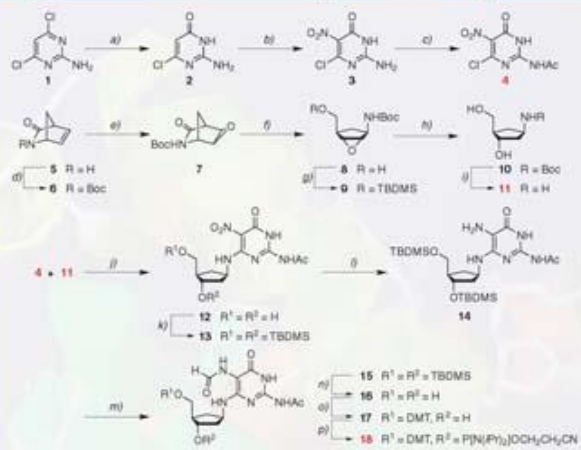
Figure 1: Geometries of FaPydG (left) and cFaPydG (right).

Structures were obtained by B3LYP/6-31G* density functional calculation with geometry optimization using Gaussian 98 (Rev. A.9)

References and Acknowledgements

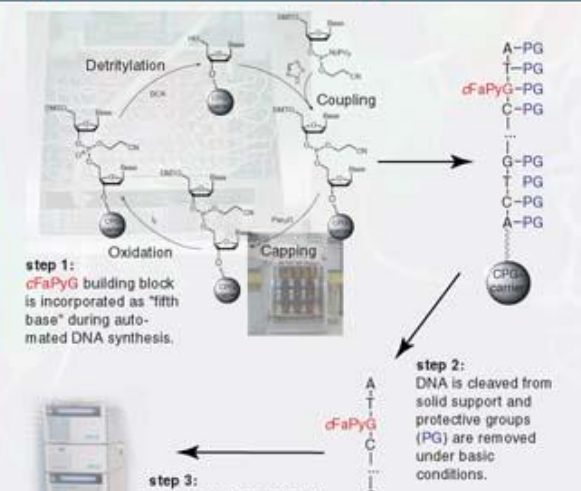
... J. Gierlich, T. Carell, *Angew. Chem. Int. Ed.*, in press.
 ... T. Carell, *Chem. Eur. J.* 2002, 8, 293.
 ... J. G. Muller, *Chem. Rev.* 1998, 98, 1109.
 ... structure was generated from 1EBM.pdb, "Crystal structure of the human B-lymphocyte (hCcp1) bound to a substrate oligonucleotide". S. D. Ammer, D. P.

Synthesis of the cFaPyG building block



a) 1 N NaOH, 100 °C, 1 h, 99%; b) HNO₃/NO₂, H₂SO₄, 0 °C, 15 min, 85%; c) Ac₂O, H₂SO₄, 90 °C, 60 min, 80%; d) Boc₂O, DMAP, THF, 25 °C, 85%; e) mCPBA, CH₂Cl₂, 25 °C, 20 h, 72%; f) NaBH₄, MeOH, 0 °C, 0.5 h, 92%; g) TBDMSCl, imidazole, DMF, 25 °C, 3 h, 90%; h) Red-AP, toluene, 25 °C, 3 h, 93%; i) H₂O, 100 °C, 14 h, 95%; j) DIPEA, DMF, 70 °C, 90 min, 72%; k) TBDMSCl, imidazole, DMF, 25 °C, 3 h, 88%; l) P₂S₅, H₂, EtOH, 25 °C, 3 h m) HCOOH, DIPEA, EDC, DMF, 25 °C, 48 h, 65% for two steps; n) HF-pyridine, pyridine, EtOAc, 25 °C, 20 h, 97%; o) DMTCL, pyridine, DMAP, 0-20 °C, 3 h, 62%; p) DIPEA, ClP(N)(Pr)₂OCH₂CH₂CN, THF, 0 °C, 30 min, 86%.

Synthesis of modified oligonucleotides



Analysis

The oligonucleotides had, after preparative HPLC purification, a purity of >98%.

A HPLC/MS/MS experiment of a total digest of the DNA proved the incorporation of cFaPydG. The fragmentation patterns of the five compounds separated during chromatography were identical to the monomeric and fully deprotected nucleotides dA, dT, dC, dG and cFaPydG.

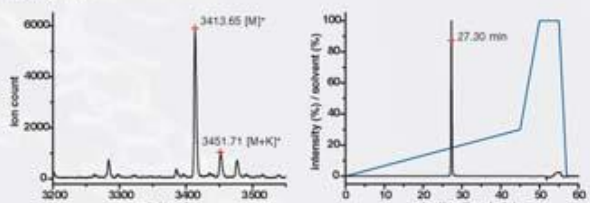


Figure 2: Analytical data of the oligonucleotide 5'-d(CGCATXTAGCG)-3'; X=cFaPyG.

Results

Three oligonucleotides containing cFaPydG, 8oxodG and dG within the same sequence have been synthesized. These strands were hybridized with their four counterstrands containing the four canonical bases as counterbases.

All mismatches strongly destabilized the duplex by at least 14 °C. The two lesions generally destabilized the strand. 8-oxodG paired relatively well with dC and dA.

5'-d(CGCATXTAGCG)-3'
 3'-d(CGCTAYATCGC)-5'

	X = dG	X = 8oxodG	X = c FaPydG
Y = dA	33.9	45.0	16.1 (54.9)
Y = dC	51.8	45.6	36.9
Y = dG	37.9	31.4	16.1 (54.9)
Y = dT	35.6	36.7	45.0

Table 1: UV-melting points of examined DNA duplexes.

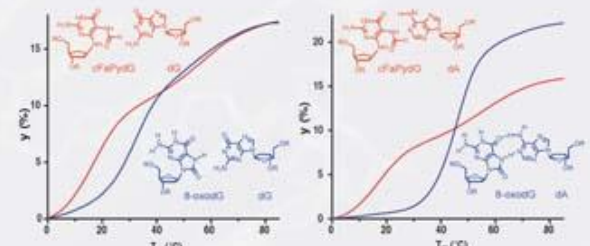


Figure 3: Melting curves of cFaPydG and 8-oxodG in complex with purine bases.



Importance of Cell-Cell Communication on VIC Activation

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MOTIVATION

Heart transplant surgeries are performed each year in the United States. Current methods of heart valve replacement use autologous human tissue that can grow and contract. Through tissue engineering, this ideal may be achieved. This has the potential to serve as an alternative to heart valve transplants.

Current Methods



Future Option



Current Methods: Autologous human tissue that can grow and contract. Through tissue engineering, this ideal may be achieved. This has the potential to serve as an alternative to heart valve transplants.

Future Option: Tissue Engineering: Synthetic heart valves that can be implanted and contract. This has the potential to serve as an alternative to heart valve transplants.

BACKGROUND

Cell-cell communication has been shown to be vital to the development of different tissues, including heart valves. Communication is made possible through signaling molecules, which are made of proteins or lipids. These molecules bind to receptors on the cell surface, which then activate the cell through gap junctions.

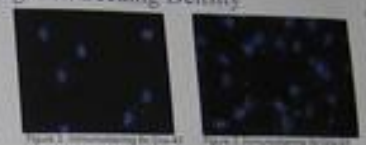
Cells that were exposed to neighboring cells showed increased activation over the course of the experiment. This suggests that cell-cell communication is important for VIC activation.

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VIC Expression of Connexin-43 with Varying Cell Seeding Density

Immunostaining

- Confirms the presence of Connexin 43 (Cx43) localized in stress around cells
- Shows increased Cx43 expression with higher cell seeding densities



Western Blot

- Seeding densities did not show a statistical difference between conditions
- Needs to be repeated to reduce error

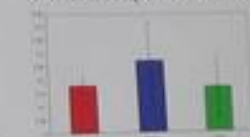


Figure 4: VIC Expression of Cx43 with Varying Cell Seeding Density

Figure 4: VIC Expression of Cx43 with Varying Cell Seeding Density. Shows increased Cx43 expression with higher cell seeding densities.

The Importance of Communication on VIC Activation

Quantitative Immunostaining

- Cells exposed to the communication enhancer lithium chloride (LiCl) and the communication inhibitor heparin
- Cells exposed to heparin show similar morphology to control cells
- Control cells are elongated and are more confluent than heparin-treated cells

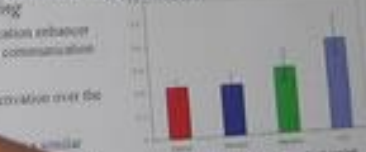


Figure 6: Importance of Communication on VIC Activation

Figure 6: Importance of Communication on VIC Activation. Shows increased activation over the course of the experiment. This suggests that cell-cell communication is important for VIC activation.

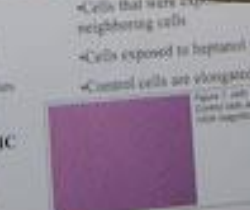


Figure 6: Importance of Communication on VIC Activation

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SUMMARY

Current results show that VICs express Cx43, suggesting that they may communicate through gap junctions. When modulators are added to increase or decrease communication, there is an increase in Cx43 expression. The correlation between cell communication and VIC activation needs to be further investigated through future work.

FUTURE WORK

- Use immunoprecipitation of VICs to further investigate communication among cells needed at varying densities in the presence of different communication modulators
- Investigate the direct effect of communication modulators on Cx43 expression using immunostaining and Western blot techniques
- Repeat immunostaining and western blot techniques to check the reliability of current results and to investigate changes of Cx43 expression with varying seeding densities and when cells are treated with communication modulators
- Repeat quantitative immunostaining experiments to compare previous results and further investigate the role of cell-cell communication to VIC activation

ACKNOWLEDGMENTS

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ABSTRACT

Network-on-chip has been proposed as an alternative to bus-based system to achieve high performance and scalability. The topology of on-chip interconnect plays a crucial role in System on chip performance, energy, and area requirements

An on-chip interconnects architecture following WK-recursive topology is proposed. WK-recursive interconnect is analyzed and compared with two networks on chip structures: 2D Mesh and Spidergon. Comparison results for performance metrics, such as the throughput, the communication load, and latency are reported. Initial results show that WK-Recursive on-chip interconnect generally outperforms the other architectures in main performance metrics

W-recursive attractive properties

A high degree of regularity, symmetry, efficient communication, and ease of extendibility that suit network on-chip infrastructures

MOTIVATION

A new architecture, based on recursive networks, is investigated. WK-recursive network was initially proposed in [2] as a network for VLSI implementation. Since this topology has many attractive properties, such as a high degree of regularity, symmetry and an efficient communication, WK-Recursive networks have also received considerable attention in parallel computing community [3]. An interesting property that makes this structure most suitable for NoC architectures is the ability to expand the network to any arbitrary size level without reconfiguring the edges. In this paper, WK-recursive network is compared with the most commonly used topologies in NoC: 2D regular mesh and Spidergon networks. Simulation results are reported for different performance metrics.

METHODOLGY AND ANALYSIS

Performance metrics are explored for the considered topologies. A simulator developed in [4] is upgraded and modified to suit different topologies and their related parameters [5]. Recently, NoC architectures have been studied and compared based on different performance metrics such as message delay, throughput and network load [1, 5, 6]. In our study, topologies of 16-nodes of 2D mesh, Spidergon, and WK(4,2) are constructed (see figure 1). WK-Recursive network with amplitude W and level L, is denoted by a WK(W,L) [3].

To analyze and compare the above interconnect topologies, the following performance metrics are considered: latency, flits loss, aggregated throughput, and communication load [4, 5]. The considered values of the injection rate are 70, 100, 130, 160, and 190Mbps. The size of the buffer is fixed to 32 flits. Figure 2 compares the latency of the three topologies when a heavy traffic is applied. In this figure, 2D mesh and Spidergon show higher maximum latency compared to the WK-recursive topology. Figure 3 shows the variation of aggregated throughput under different injection rates. WK-recursive interconnect outperforms the rest of the topologies when the injection rate is less than 160Mbps because of lower loss rate as depicted in figure 4. Figure 5 shows that WK outperforms the rest of topologies in the communication load.

WK-recursive Network: An overview

The communication between processors was the key issue to many parallel algorithms. It was considered as one of the most important issues for interconnection networks. It is known that the topology plays a crucial role to address this issue. Several topologies, such as Mesh and 2D torus have been proposed in the field of parallel computing and adopted in NoC research [5]. Recently, an attractive topology called WK-recursive network has received considerable attention in parallel computing due to its many favorable properties, such as high degree of regularity, symmetry and efficient communication, scalability, and ease of extendibility [4]. This topology has been initially proposed for VLSI implementations [1] and later adapted as a network topology for parallel computing [2, 3, 4].

One of the interesting properties of this structure is its ease of expandibility; the WK-recursive network can be constructed hierarchically by grouping basic modules. More precisely, a WK-recursive network with amplitude W and level L, denoted by a WK(W,L), can be recursively constructed. A WK(W, 0) is a vertex with W free edges. A WK(W, 1) is a W-vertex complete graph that is denoted by a KW. Each vertex has one free edge and W-1 edges that are used for connecting to the other vertices. A WK(W, H) consists of W copies of WK(W, H-1) as supervertices and the W supervertices are connected as a KW, where. By induction, WK(W,L) has WL vertices and W free edges. Consequently, for any specified degree W, WK-Recursive networks can be expanded to an arbitrary level L without reconfiguring the edges. The structures of a WK(4, 0), a WK(4, 1), and WK(4, 2) are depicted in figure to the right.

RESULTS

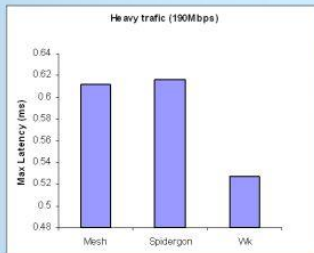


Figure 2. Maximum latency for the three topologies.

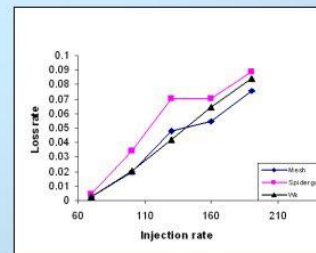


Figure 2. Variation of loss rate vs. injection rate

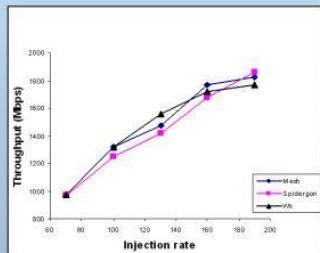


Figure 3. Variation of throughput vs. injection rate

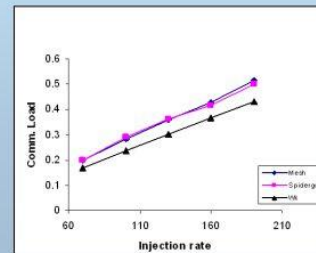
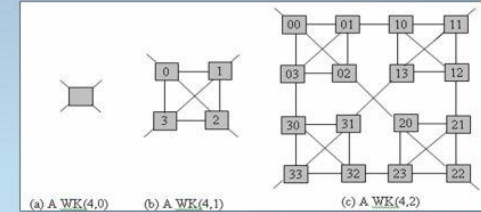


Figure 5. Variation of communication load vs. injection rate



The structures of (a) WK(4, 0), (b) WK(4, 1), and (c) WK(4, 2)

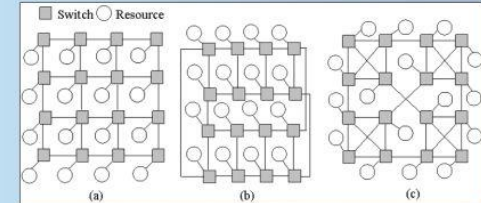


Figure 1. NoC Topologies on the chip layout: (a) 2D Mesh, (b) Spidergon, (c) WK

CONCLUSIONS

We proposed a NoC interconnect based on the WK recursive network. A simulation study aimed at exploring this on-chip interconnect for NoC is conducted. The study compares this topology with two NoC architectures: 2D regular mesh and Spidergon. Selected configurations of these architectures have been constructed and simulated to compare main performance metrics such as packet losses, throughput, message delay, and network load. WK-recursive interconnect generally outperforms Mesh and Spidergon topologies because of its regular and stable behavior at the nodes' level, since it has lower latency and lower communication load. However, when heavy traffic is applied a slight increase in drop probability is appearing. Other important metrics, such as energy consumption and area requirements, is an ongoing work.

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Site Characterization Projects for Contaminant Hydrogeology



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Motivations for the project

- Synthesis of geologic, hydrologic and contaminant data
- Examples of data available for actual sites
- Data uncertainty
- Data gaps
- Multiple and differing interpretations

Other Essential Data

- Water level data (from multiple years or seasons if possible)
- Contaminant concentration data (from sampling rounds at similar times as water levels)

Hydro Chemical Table 2 - Water level data 1998 and 2003 data

Well No.	Date	Time	1998		2003	
			Depth to Groundwater (ft)	Water Surface Elev. (ft)	Depth to Groundwater (ft)	Water Surface Elev. (ft)
W1	08/05/98	11:30	2.4	11.5	1.5	11.5
W2	08/05/98	11:30	2.8	11.5	1.8	11.5
W3	08/05/98	11:30	3.2	11.5	2.2	11.5
W4	08/05/98	11:30	3.6	11.5	2.6	11.5
W5	08/05/98	11:30	4.0	11.5	3.0	11.5
W6	08/05/98	11:30	4.4	11.5	3.4	11.5
W7	08/05/98	11:30	4.8	11.5	3.8	11.5
W8	08/05/98	11:30	5.2	11.5	4.2	11.5
W9	08/05/98	11:30	5.6	11.5	4.6	11.5
W10	08/05/98	11:30	6.0	11.5	5.0	11.5

Hydro Chemical Table 1 - Concentration Data

Well No.	Date	Time	1998		2003	
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W1	08/05/98	11:30	2.4	11.5	1.5	11.5
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W4	08/05/98	11:30	3.6	11.5	2.6	11.5
W5	08/05/98	11:30	4.0	11.5	3.0	11.5
W6	08/05/98	11:30	4.4	11.5	3.4	11.5
W7	08/05/98	11:30	4.8	11.5	3.8	11.5
W8	08/05/98	11:30	5.2	11.5	4.2	11.5
W9	08/05/98	11:30	5.6	11.5	4.6	11.5
W10	08/05/98	11:30	6.0	11.5	5.0	11.5

Checklists for assessing and comparing groups

Students	Comparison	1	2	3	4
Water level map					
Contaminant +1.5D map					
Geologic cross-section					
Geologic cross-section and labels					
3D map					
Scale of depression (1:500)					
Other features					

Background Information Provided to Students

• History of suspected source and/or detected plume
Chips 'N Dips (CND) Corporation has been attempting to develop silicon wafers as a snack treat. Unfortunately, during the early stages of product development and manufacturing, housekeeping operations at the plant were rather careless and a number of TCE spills occurred. By the time a groundwater plume was discovered in 1983, it had moved beyond the CND property boundary.

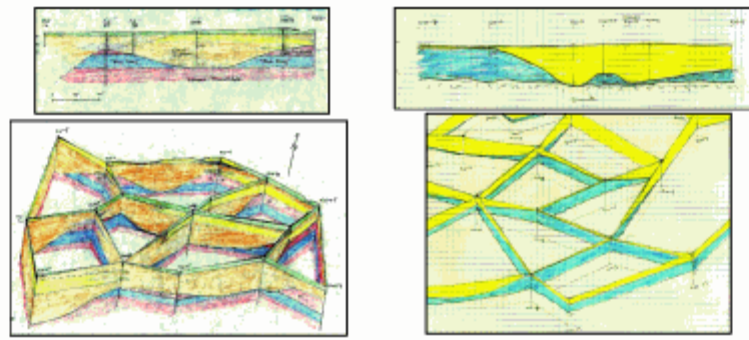
• Critical questions to be answered by student "consultants"
It is now early 2004 and you have been called in as a consultant to assess the effectiveness of the existing remedial measures at the site and to recommend additional measures if necessary.

Regional geologic and hydrogeologic setting



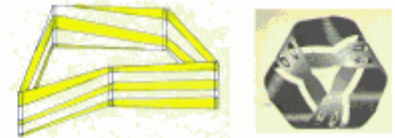
Interpretive Documents

- Geologic/hydrostratigraphic cross sections and a fence diagram



Useful Lessons 1

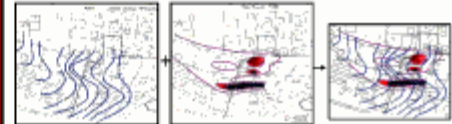
3D interpretations should be geologically reasonable



What's wrong with this fence diagram?

Useful Lessons 2

Water level and dissolved plume maps should be generally consistent



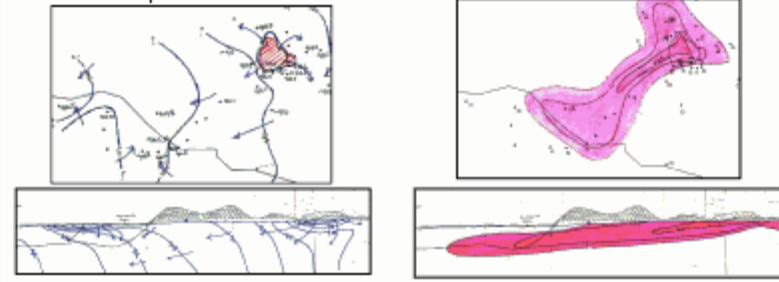
Data Set for Student Interpretation

- Geologic/geotechnical boring logs from monitoring wells (nested if possible) and nearby private or municipal wells
- Base Map



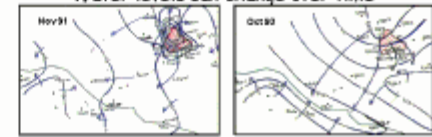
Additional Interpretive Documents

- Water level maps and cross section
- Plume maps and cross sections



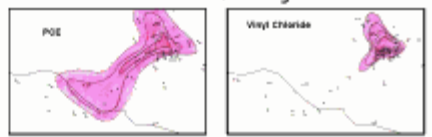
Useful Lessons 3

Water levels can change over time



Useful Lessons 4

Retardation and/or Degradation



Note: Examples in this poster are from a number of different site projects that have been



SCIENTISTS, RECORDS, AND THE PRACTICAL POLITICS OF INFRASTRUCTURE:

AN ETHNOGRAPHIC EXPLORATION OF DOCUMENTATION IN SCIENCE

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BACKGROUND

SCIENCE AND WRITING ARE INEXTRICABLY BOUND. SCHOLARS HAVE PAID A GREAT DEAL OF ATTENTION TO WRITING IN SCIENCE, PARTICULARLY THE ACT OF FORMAL WRITING AND PUBLICATION AS THEY CONSTITUTE TO KNOWLEDGE PRODUCTION AND ORGANIZATION, BUT FORMAL PUBLICATION IS ONLY ONE SITE OF INTERSECTION BETWEEN SCIENCE AND THE PRODUCTION OF TEXTS. OTHER KINDS OF WRITING, PARTICULARLY RECORDS OF DAILY RESEARCH, CONSTITUTE THE BULK OF SCIENTIFIC DOCUMENTATION, AND YET THERE IS A TAKEN-FOR-GRANTED QUALITY AND A LACK OF ARTICULATION AROUND THE ISSUE OF RECORDKEEPING. BECAUSE RECORDKEEPING IS DESIGNED TO SUPPORT OTHER TASKS, EXERCISING TIME AND SPACE TO ALL NEEDS OF MODERN SCIENTIFIC PRACTICE, AND IS SO THOROUGHLY EMBEDDED IN THAT PRACTICE, IT HAS TAKEN ON THE TRANSPARENCY OF ALL SUCCESSFUL INFORMATION INFRASTRUCTURES.

THE PURPOSE OF THIS DISSERTATION HAS BEEN TO UNDERSTAND HOW THESE STANDARDS ARE REFERED AND INTERPRETED IN A SCIENTIFIC COMMUNITY OF PRACTICE. TO "SHINE OPEN THE INFRASTRUCTURE," I HAVE BEEN CONDUCTING A DISSERTATION STUDY TO EXAMINE HOW ONE PARTICULAR WORKGROUP OF SCIENTISTS CREATED RECORDS, THE NATURE OF THEIR DOCUMENTS, AND THE WAYS TO WHICH THEY PUT THESE RECORDS.

RESEARCH DESIGN

RESEARCH QUESTIONS

- WHAT IS THE NATURE OF THE RECORDS CREATED IN A COMMUNITY OF SCIENTIFIC PRACTICE?
- HOW DO THESE SCIENTISTS ORGANIZE, MANAGE, AND ACCESS RECORDS?
- HOW ARE INFORMATION ORGANIZATION AND RECORDS IN THE SOCIAL SCIENCE?

CONDUCT PARTICIPANT-OBSERVER STUDY IN BASIC RESEARCH ACADEMIC LABORATORY

- THE LABORATORY CONSISTS OF A RESEARCH ORGANIZATION THAT IS INTERDISCIPLINARY AND COLLABORATIVE IN NATURE.
- PARTICIPANT-OBSERVER RESEARCH INVOLVES OBSERVING AND INTERACTING WITH MEMBERS OF THE COMMUNITY OF PRACTICE AND PARTICIPATING IN THEIR COMMUNITARIAN AND SCIENTIFIC ACTIVITIES.

CONDUCT OPENENDED INTERVIEWS WITH MEMBERS OF LABORATORY

ANALYZE SAMPLES OF LABORATORY DOCUMENTS AND RECORDS TO OBSERVE PATTERNS AND GENERATE TYPOLOGY

SIGNIFICANCE

THIS INTERMEDIARY RESEARCH PROJECT SUPPORTS A NUMBER OF RESEARCH REASONS, BOTH APPLIED AND THEORETICAL. UNDERSTANDING HOW AND WHY SCIENTISTS KEEP RECORDS, THE QUALITY THEY ASSESS TO OWN, AND THE WAYS OF RECORDS IN THE PRODUCTION OF SCIENCE HAS IMPACT FOR ARCHIVAL STUDIES, INFORMATION SCIENCE, AND SCIENCE STUDIES.

MORE SPECIFICALLY, RECORDKEEPING IS A TECHNOLOGY OF POWER. AS IT IS USED TO DOCUMENT AN ORGANIZATION, SOME VIEWPOINTS BECOME CENTRAL WHILE OTHERS BECOME MARGINALIZED. WE NEED TO UNDERSTAND HOW AND WHY THIS KNOWING BECOMES ORGANIZED IN SUCH AN ORGANIZATIONAL PART OF OUR ENVIRONMENT LIFE, IT IS NECESSARY FOR US TO UNDERSTAND THAT WHICH IT TAKES TO BE CREATED.

PRELIMINARY FINDINGS

- TENSIONS BETWEEN COMMUNITY AND INSTITUTIONAL STANDARDS FOR SCIENTIFIC RECORDKEEPING AND LOCAL PRACTICES. THESE MANIFESTS ITSELF IN POTENTIAL LARGES OF COMMUNICATION AND ORGANIZATION BETWEEN FUNDING AGENCIES, PRINCIPAL INVESTIGATORS, JUNIOR RESEARCHERS, AND STUDENTS. IT IS ALSO A FUNDAMENTAL PARADOX OF INFORMATION INFRASTRUCTURE.
- SCIENTIFIC RECORDS ARE "LIMINAL," THE NATURE OF THE RECORDS IS NOT "BUILT" IN AN ADVANCE AND ACCUMULATED IN THE WAY ARCHIVISTS CREATE AND MANAGE THEIR OWN RECORDS.
- WHILE LABORATORY RECORDS AND DOCUMENTS SERVE AS ADMINISTRATIVE MEMORY, THEY PLAY MANY OTHER ROLES - INCLUDING DOCUMENTING THE GROWTH OF THE SELF AS SCIENTIST, ESTABLISHING AGENCY OVER THE ENVIRONMENT, AND MEDIATING BETWEEN INTERNAL TO THE SCIENTIST AND EXTERNAL FROM THE COMMUNITY AND INSTITUTIONAL STANDARDS OF ACCOUNTABILITY.

FUTURE RESEARCH

TO PUT THIS RESEARCH INTO A LARGER POLICY CONTEXT, I WILL BE CONDUCTING INTERVIEWS WITH SENIOR ADMINISTRATORS AND OFFICIALS AT NATIONAL AGENCIES THAT FUND AND CHARGE BIOLOGICAL RESEARCH, THE NATIONAL INSTITUTES OF HEALTH AND THE OFFICE OF RESEARCH INTEGRITY, DEPARTMENT OF HEALTH AND HUMAN SERVICES. TOPICS THAT I WILL EXPLORE INCLUDE:

- IMPACT AND IMPLICATIONS OF THE FREEDOM OF INFORMATION ACT (FOIA)
- DATA AND LABORATORY AUDITING PRACTICES
- ETHICS TRAINING OF SCIENTISTS
- RELATIONSHIP BETWEEN NIH/ORE AND THE RESEARCHERS THAT ARE FUNDED
- INSTITUTIONAL PERSPECTIVES ON RECORDS CREATION AND MANAGEMENT

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亚克力底写真喷绘饰面

标准展架

蓝色亚克力饰面

ICC 2008, BEIJING, CHINA
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2008世界通信大会

Height=1.5m

1m

0.5m

Height=0.75m







remain poorly understood (Oishi, 2003; Huber, 2003). The Evi/VASP protein family is implicated in regulation of neurite extension during growth cone guidance (Lemon, 1999; Tappin, 2001) and is a potential Evi/VASP binding partner which is specifically expressed in the nervous system (Bost, 2002). Their potential interaction was originally identified through a yeast two-hybrid screen followed by localization experiments.

Biochemical



Figure 1. Model for DCC-Evi-VASP interactions. Image from Bost et al. (2002).



Figure 2. The DCC-Evi-VASP complex. Multiple Evi/VASP protein molecules bind to the cytoplasmic tail of DCC. The DCC-Evi-VASP complex is specifically expressed in the nervous system. Image from Bost et al. (2002).

Localization

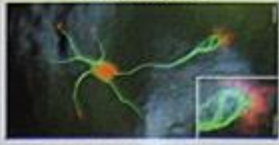


Figure 3. The cytoplasmic tail of a developing zebrafish embryo shows a complex of DCC-Evi-VASP (red) and Evi-VASP (blue). Image from Bost et al. (2002).

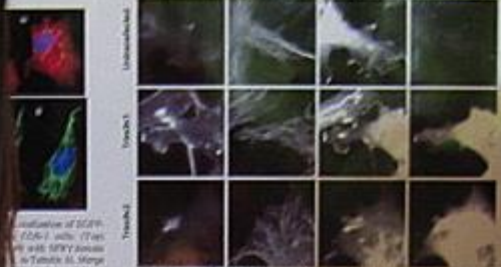


Figure 4. Localization of DCC-Evi-VASP complex in zebrafish. DCC-Evi-VASP (red) and Evi-VASP (blue) are localized to the cytoplasmic tail of DCC in the limb/fin bud, trophoblast, and trophoblast. Image from Bost et al. (2002).



Figure 5. DCC-Evi-VASP complex in zebrafish. DCC-Evi-VASP (red) and Evi-VASP (blue) are localized to the cytoplasmic tail of DCC in the limb/fin bud, trophoblast, and trophoblast. Image from Bost et al. (2002).



Figure 6. DCC-Evi-VASP complex in zebrafish. DCC-Evi-VASP (red) and Evi-VASP (blue) are localized to the cytoplasmic tail of DCC in the limb/fin bud, trophoblast, and trophoblast. Image from Bost et al. (2002).



Figure 7. DCC-Evi-VASP complex in zebrafish. DCC-Evi-VASP (red) and Evi-VASP (blue) are localized to the cytoplasmic tail of DCC in the limb/fin bud, trophoblast, and trophoblast. Image from Bost et al. (2002).

Conclusions

- Yeast two hybrid results suggest that a segment of Trim9 could interact with Evi and the cytoplasmic tail of DCC.
- Full length proteins may not allow access to binding sites exposed in truncated versions
- Parts of Trim9 could be poorly expressed or toxic to yeast
- Trim9 is expressed specifically in the nervous system and localizes to microtubules in primary cortical neurons
- We hypothesize that Trim9 interact with Evi-VASP proteins when they are localized to filopodia during axon guidance

DCC/T9
DCC/T9
DCC/T9
EVL/A
EVL/A
EVL/A
EVL/A
EVL/A
EVL/A

MIT Summer Research Program 2006
Leticia Medina

MIT Summer Research Program 2006
Leticia Medina
MIT

Introduction

Low Flow Fuel Cell System Characteristics

Low flow fuel cells are designed for applications where power density is not the primary concern, but where long life and low maintenance are critical. These cells are typically used in remote or inaccessible locations where refueling is difficult.



The fuel cell system is designed to operate at a low flow rate, which allows for a longer life and lower maintenance. The system is also designed to be compact and lightweight, making it suitable for use in remote or inaccessible locations.



Setup

The fuel cell system is set up in a laboratory environment. The system is connected to a power supply and a load resistor. The fuel cell is operated at a constant current and the voltage is measured across the load resistor.



Method

The fuel cell system is operated at a constant current and the voltage is measured across the load resistor. The current is varied and the voltage is measured for each current value. The resulting data is plotted as a graph of voltage versus current.



Results



Conclusion

The fuel cell system is designed to operate at a low flow rate, which allows for a longer life and lower maintenance. The system is also designed to be compact and lightweight, making it suitable for use in remote or inaccessible locations.

The Future

The fuel cell system is designed to operate at a low flow rate, which allows for a longer life and lower maintenance. The system is also designed to be compact and lightweight, making it suitable for use in remote or inaccessible locations.

The fuel cell system is designed to operate at a low flow rate, which allows for a longer life and lower maintenance. The system is also designed to be compact and lightweight, making it suitable for use in remote or inaccessible locations.



The fuel cell system is designed to operate at a low flow rate, which allows for a longer life and lower maintenance. The system is also designed to be compact and lightweight, making it suitable for use in remote or inaccessible locations.

References

1. Fuel Cell Handbook, 6th Edition, NREL, 2003.

2. Fuel Cell Handbook, 5th Edition, NREL, 2000.

Table 1

Current (A)	Voltage (V)
0.0	1.0
0.2	0.9
0.4	0.8
0.6	0.7
0.8	0.6
1.0	0.5

Table 2

Current (A)	Voltage (V)
0.0	1.0
0.2	0.9
0.4	0.8
0.6	0.7
0.8	0.6
1.0	0.5

Figure 1

A photograph of the fuel cell system setup, showing the fuel cell stack, power supply, and load resistor. The setup is placed on a table, and the connections are clearly visible.



Low Flow Flush Valve Development Success



Early Board Installation

• Installation of the flush valve in the early stages of the project...

Timeline

• The project timeline shows a steady progress from the initial design phase...

Timeline

• The project timeline shows a steady progress from the initial design phase...

The Early Flush Valve



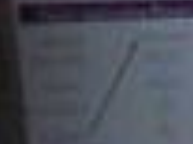
Timeline & Cost

• The timeline and cost analysis shows a significant reduction in expenses...

Timeline & Cost

• The timeline and cost analysis shows a significant reduction in expenses...

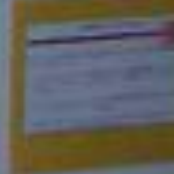
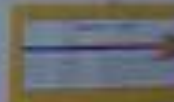

The Early Flush Valve



Timeline & Cost

• The timeline and cost analysis shows a significant reduction in expenses...

Timeline & Cost





Colaborators



Masahiko ISOBE



- **Dr. Masao ARAI**

- Senior Researcher, Computational Materials Science Center, NIMS
- *ab-initio* band calculation



- **Dr. Mitsuyuki SHIZUYA**

- Post Doctoral Fellow, Advanced-Nano Materials Laboratory, NIMS
- Synthesis and physical properties measurements
- (Present Address: TDK Co., Ltd.)



- **Dr. Eiji TAKAYAMA-MUROMACHI**

- Managing Director, Advanced-Nano Materials Laboratory, NIMS







Metallic oxide coating of Ti for DSA used in chlorine production for water chlorination

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¹Faculty of Metallurgical Engineering and Environmental Protection, University of Medicine and Pharmacy, Bucharest, Romania
²Faculty of Chemistry, University of Medicine and Pharmacy, Bucharest, Romania

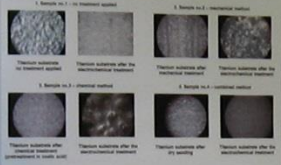
Introduction

The most widely used water disinfectant is chlorine. Chlorine disinfection is based on oxidation, therefore it should be obtained on-site and systems to keep it specific systems. For example, instead of bringing water with a relatively high concentration of chlorine to treatment plants, chlorine is no longer stored and transported (as it is generated from saline solution only if needed), in small quantities and is immediately injected into the water pipe and the chlorine concentration is kept constant along the water system instead of decreasing toward the end-user.

The graphite anodes used in the past for chlorine production was replaced with dimensionally stable anodes (DSA) that was developed in 1989 by Harsco Corporation. DSA consists of a titanium metal (or titanium coated with niobium oxide film). A large variety of coating compositions and thicknesses can be obtained, with different properties electrocatalytic activity, life span, corrosion resistance to various environments, etc. Therefore the DSA can be customised for specific applications. A very important process in the substrate preparation, as its surface must be suitable to allow its work properly. Several methods are comparatively investigated (mechanical, chemical and combined methods). The quality of prepared substrate surface is investigated by PSC, electrochroming and by the adherence, homogeneity and uniformity of PSC, depend on a number of prepared substrate surface quality.

Results and discussion

1. Quality of prepared substrate surface



2. Voltage (V) dependence on time (t) for the 4 samples at PSC electrochroming

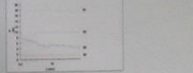


Figure 1. Voltage (V) dependence on time (t) for the 4 samples at PSC electrochroming

Technology for metallic oxide coating of titanium for DSA used in chlorine production for water chlorination



4. The figure presents the polarization curves for titanium substrate coated with RuO₂/TiO₂ at different values RuO₂/TiO₂ composition & constant anodic scan rate 100 mA/cm² at 70 °C in 10 g/l NaCl solution (pH=2, at 80 °C)

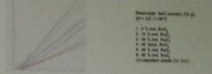


Figure 2. Polarization curves for titanium substrate coated with RuO₂/TiO₂ at different values RuO₂/TiO₂ composition & constant anodic scan rate 100 mA/cm²

5. Table 1. Tafel's coating composition for the electrochroming anodes: RuO₂/TiO₂/SnO₂

Sample	RuO ₂ (wt%)	TiO ₂ (wt%)	SnO ₂ (wt%)
A	10	90	0
B	20	80	0
C	30	70	0
D	40	60	0
E	50	50	0
F	60	40	0
G	70	30	0
H	80	20	0
I	90	10	0
J	100	0	0



Figure 3. Polarization curves for anodes with RuO₂/TiO₂/SnO₂ coating

6. Table 2. Deposited samples and anodic quality for anodes with electrochroming RuO₂/TiO₂/SnO₂

Sample	Area (cm ²)	Current (mA)	Potential (V)	Time (min)	Quality
A	1.0	10	1.5	10	Good
B	1.0	20	1.5	10	Good
C	1.0	30	1.5	10	Good
D	1.0	40	1.5	10	Good
E	1.0	50	1.5	10	Good
F	1.0	60	1.5	10	Good
G	1.0	70	1.5	10	Good
H	1.0	80	1.5	10	Good
I	1.0	90	1.5	10	Good
J	1.0	100	1.5	10	Good

Conclusions

If the results obtained by several methods were compared and the best method for surface preparation was selected - it's important to know that the prepared substrate was coated with a metallic oxide film. Several film compositions (RuO₂/TiO₂ and RuO₂/TiO₂/SnO₂) in various ratios, deposited directly on Ti were investigated. The electrochroming procedure of these coatings was evaluated by plotting the polarization curves of chlorine fabrication from saline solution. In the range of obtained results, we also investigated the best results were compared and the best method for surface preparation was selected. The best results were compared and the best method for surface preparation was selected. The best results were compared and the best method for surface preparation was selected.



Hybrid inorganic-organic polymer composites for polymer-electrolyte fuel cells

Andrea Ambrosini

Cy Fujimoto, Ron Stanis, Chris Cornelius

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INTRODUCTION

Polymer Electrolyte Membranes (PEM) Fuel Cells

PEM fuel cells are currently the leading candidate for battery replacement in portable electronics and stationary applications. One of the primary technical challenges of PEMs is their poor performance at low relative humidities due to poor proton transport in the polymeric electrolyte. Revenues of these fuel cell systems are high, but only organic polymer membranes can operate only at temperatures $<100^\circ\text{C}$. The development of polymer electrolytes that can operate between $120\text{--}150^\circ\text{C}$ and at lower relative humidities will result in more efficient fuel cell systems.

Current State of the Art Membranes: Nafion

Structure:
- Sulfonic acid groups
- Fluoropolymer backbone
- Polymer matrix (Nafion)
- Material cost (\$/kWatt)
- Durability (cycles/starts result in loss of proton conductivity)
- High proton conductivity
- Good mechanical properties
- Long life cell lifetime

Sulfonated Diels-Alder Poly(Phenyls) (SDAPP)

Structure:
- Sulfonated Diels-Alder Poly(Phenyls)
- High proton conductivity
- Good mechanical properties
- Long life cell lifetime
- Material cost (\$/kWatt)
- Durability (cycles/starts result in loss of proton conductivity)
- High proton conductivity
- Good mechanical properties
- Long life cell lifetime

Heteropolycids (HPA)

Structure:
- Heteropolycids (HPA)
- High proton conductivity
- Good mechanical properties
- Long life cell lifetime
- Material cost (\$/kWatt)
- Durability (cycles/starts result in loss of proton conductivity)
- High proton conductivity
- Good mechanical properties
- Long life cell lifetime

Hybrid Organic-Inorganic Composites

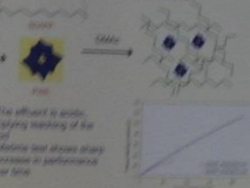
Combine the best characteristics of organic polymers with the high temperature stability, conductivity, and functionality of inorganic heteropolycids.

Increased temperature stability
Improved water retention
Improved conductivity
Lower mechanical strength

SYNTHESIS AND CHARACTERIZATION

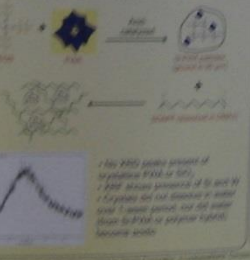
First Approach

Physical incorporation of HPA into polymer by co-casting from a DMAc solution



Second Approach

Synthesis of SiO₂-PWE particles followed by physical incorporation of particles into film



Second Approach (continued)



The use of HPA particles can be...
- HPA between 1.6 - 2.2 nm
- Water uptake between 20-30% (200% water uptake)
- Loading of SiO₂-PWE particles not observed for HPA
- Heteropolycids do not increase conductivity but increase mechanical strength

Third Approach

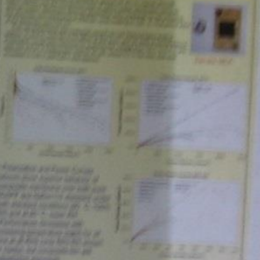
In situ synthesis of silica contents within polymer
- HPA can be fully incorporated, but not homogeneous in appearance
- No HPA loading

PROPERTIES

Conductivity



Fuel Cell Tests



CONCLUSIONS

Summary
- HPA incorporation results in improved conductivity of PEM fuel cells
- HPA incorporation results in improved mechanical strength of PEM fuel cells
- HPA incorporation results in improved water uptake of PEM fuel cells
- HPA incorporation results in improved durability of PEM fuel cells

Future Work

Develop alternative HPA structures
Develop alternative HPA structures
Develop alternative HPA structures

Acknowledgments

Support from Sandia National Laboratories
Support from Sandia National Laboratories
Support from Sandia National Laboratories



Thin Protective Coating of ZnO Using Atomic Layer Deposition

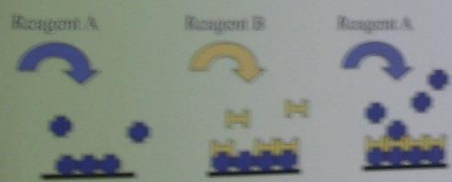
Margaret E. Welk, Robert K. Grubbs, Andrea Ambrosini
Sandia National Laboratories
Albuquerque, NM 87185

Abstract

In gas separations, sulfur impurities such as SO₂ and H₂S in the ppm level will poison functional separation membranes made of metal (Pt) and many metal oxide materials. ZnO is a well known sulfur sorbent that is converted in the process to ZnS. Using Atomic Layer Deposition we have coated a membrane support with ZnO as a protective layer. The effect of cycling between ZnO and ZnS on the morphology of the thin layer of sorbent material is studied.

Atomic Layer Deposition

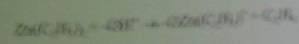
- Sequential exposure to reagents
- Each reagent chemisorbs to surface but not to itself to create a monolayer



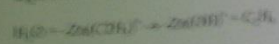
Fine control over layer thickness to atomic scale
Excellent at conformally coating high aspect ratio structures

To form the ZnO layer, we cycled between Dimethyl Zinc [Zn(CH₃)₂] and water at 200 °C.

DZG half reaction:



H₂O half reaction:



(* - surface species)

Characterization of as Prepared Samples

We deposited 450Å of ZnO on a γ-Al₂O₃ mesoporous disk support (average pore diameter is 1.8 μm).



BET

The coated support has a surface area of 1.19 ± 0.05 m²/g, whereas the uncoated support has a surface area of 1.65 ± 0.04 m²/g.

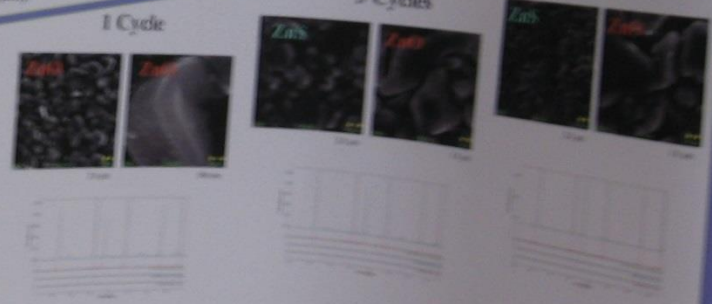


SEM

The globular Al₂O₃ support is uniformly coated. No crystalline facets are apparent.

Sulfur Uptake

While ZnO scavenges sulfur readily, the phase change and corresponding lattice parameter change between ZnO and ZnS leads to discrepancy in solid pellets. To investigate the effect of cycling on the thin ZnO coated supports, several ZnO coated supports were placed in a furnace and heated to 500 °C at a ramp rate of 1 degree per minute. The supports were exposed to 2% H₂S in N₂, flowing at a rate of 1 to 5 mL/min for 4 hours, then the gas was switched to air for 15 hours. This cycle was repeated 7 times. Samples were taken for analysis after one cycle, three cycles, and seven cycles.



The first conversion to ZnS results in crystalline formation visible in the SEM. Blending increases visibility in the third and seventh cycle images. XRD shows complete conversion between ZnO and ZnS.

Acknowledgments

The authors wish to thank DOE (DE-FC02-01-OR-21400) program for funding.

Conclusions

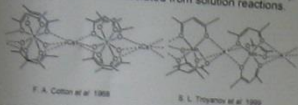
While crystalline layer increases over several generations of the porous support, porous layer of ZnO material is excellent coating of ZnS and the need to produce sensitive membrane does not require poisoning.

Heterometallic β -Diketonates as Potential Single-Source Precursors for Oxide-Based Materials

Evgeny V. Dikarev*, Haitao Zhang and Bo Li
Department of Chemistry, University at Albany

Introduction

Although heterometallic β -diketonates are promising precursors for multimetallic oxides, they are rare species due, in part, to chelating character of the ligand. Since 1960s, only a limited number of heterometallic β -diketonates have been isolated from solution reactions.

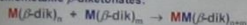


The focus of our investigation was to develop a simple high-yield synthetic approach to heterometallic main group-transition metal β -diketonates.

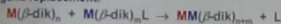
Synthetic Strategy

We suggested several low-temperature synthetic routes that appear to be general for preparation of heterometallic diketonates incorporating a wide range of s-, p-, d-, and f-metals.

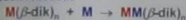
Interaction between coordinatively unsaturated homometallic β -diketonates:



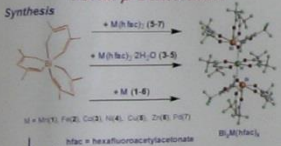
Ligand replacement:



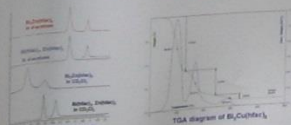
Redox reaction:



Heterometallic Bismuth-Transition Metal β -Diketonates



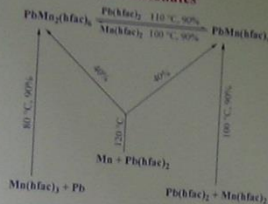
Solution and Thermal Behavior of B₂M(hfac)₄



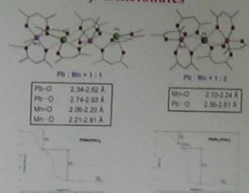
Heterometallic β -diketonate molecules retain their trimeric structure in noncoordinating solvents and dissociate in coordinating solvents.

Decomposition begins at 80-90 °C and completes at 300-350 °C showing no apparent loss of β -diketonates to sublimation.

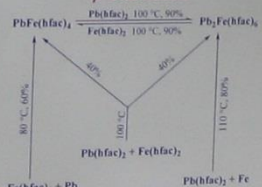
Controlled Syntheses of Pb-Mn β -Diketonates



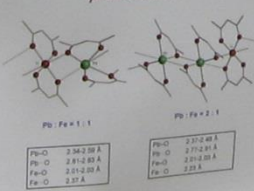
Pb(II)-Mn(II) Heterometallic β -Diketonates



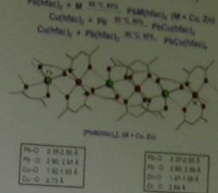
Controlled Syntheses of Pb-Fe β -Diketonates



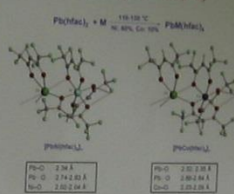
Pb(II)-Fe(II) Heterometallic β -Diketonates



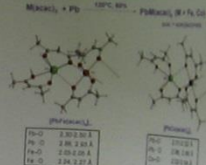
PbM(hfac)₄ (M = Cu, Zn)



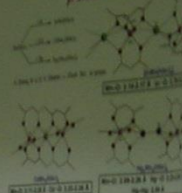
PbM(hfac)₄ (M = Co, Ni)



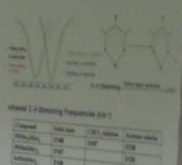
Non-Fluorinated Heterometallic β -Diketonates



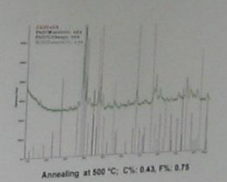
Heterometallic Manganese β -Diketonates



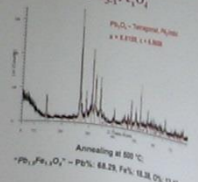
IR Study of Heterometallic β -Diketonates



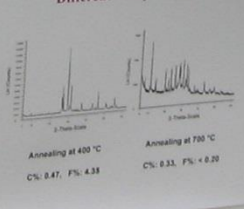
Decomposition of PbNi(hfac)₄; New Pb-Ni-O Phase



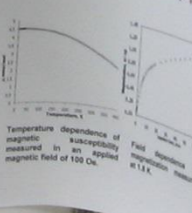
Decomposition of PbFe(hfac)₄; Pb₃Fe₂O₇



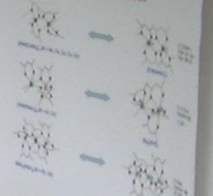
Decomposition of PbNi(hfac)₄ at Different Temperatures



Magnetic Study of Pb₃Fe₂O₇



Structural Analogy with Homometallic β -Diketonates



Summary

- A number of heterometallic β -diketonates incorporating main group and transition metals have been isolated. The structures and their structural analogies in the species in coordinating solvents.
- Heterometallic β -diketonates were built on Lewis acid-base noncoordinating solvents and dissociate into homometallic β -diketonates in coordinating solvents.
- Heterometallic β -diketonates retain their structure in noncoordinating solvents and dissociate into homometallic β -diketonates in coordinating solvents.
- Heterometallic β -diketonates with different metal ions can be obtained using different starting materials.
- Thermal decomposition of heterometallic β -diketonates results in new bimetallic oxides that cannot be obtained from high-temperature synthesis.

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ACF-PPF, 1421-0106



INTRODUCTION

The kinetics of the hydrogen evolution reaction (HER) has been intensively studied due to its importance in practical applications such as water electrolysis, chloro-alkali electrolysis and electrochemical reduction of organic compounds. The highest activity for the HER is shown by the platinum group metals; however the researchers have been focused towards the development of new materials, less expensive but with similar activity. Among these metals, nickel exhibits good corrosion resistance in aggressive environments and catalytic activity for the HER. The electrochemical activity can be further enhanced by increasing the real surface area of the electrode using the porous activity of the electrode material. One of the common ways to enlarge the real surface area is the utilization of Raney-type alloys from which the active component (Al, Zn) is dissolved by alkaline leaching. Various techniques have been developed for the preparation of the electrodes, consisting in electrodeposition of Raney-nickel powder with nickel, powder pressing of Raney-nickel, electrodeposition of Ni-Zn alloys and thermal spraying of wires or powders.

AIM

The aim of the present work is to investigate the kinetics of HER on Raney Ni and NiTi electrodes using potentiostatic steady state and electrochemical impedance spectroscopy (EIS). The electrodes used in the present study were prepared by thermal spraying of a Ni, respectively NiTi wire together with an Al wire, providing aluminium content in the coating, which is further removed by the leaching.

METHODS

Electrode preparation: Thermal spraying technique was used to obtain two types of Raney Ni electrodes: Ni electrode two different wires have been used: Ni (99.2% Ni) and Al (99.9% Al). During the thermal spray the arc current and voltage were set to 200 A and 20 V, respectively 32 V. The Raney NiTi electrodes were obtained using a NiTi wire (97% Ni, 3% Ti) and an Al wire (99.9% Al). The spraying parameters were set to 180 A and 20 V in both cases. The spraying distance ranged between 30 and 70 mm and the atomizing gas (air) pressure was 1.7 bar. After the deposition the coatings had a thickness of maximum 1 mm. Disk shaped samples with a diameter of 10 mm were cut out from the coated steel plates. In order to remove the Al from the coating, the samples were subjected to alkaline leaching in 1 M NaOH solution at about 60°C, for 2 hours. After the dissolution of Al the samples were cleaned for 10 minutes in an ultrasonic bath and further they will be referred to as Raney-nickel.

RESULTS AND DISCUSSION

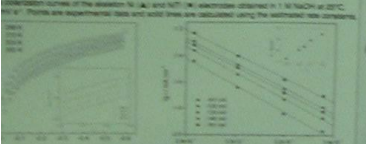
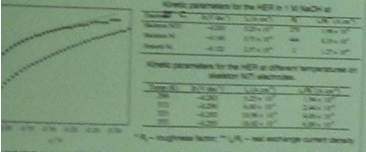
Results of the EDX analysis

Coating	Ni, wt%	Al, wt%	Ti, wt%	Si, wt%
NiTi electrode	98.5	24.9	0.2	0
Ni electrode	96.2	1.5	0.2	0
NiTi electrode	96.2	10.1	0.8	0.8
Ni electrode	97.7	2.9	0.3	0.4



SEM micrographs of the surface (a) and cross section (b) of the Raney Ni electrode after alkaline leaching.

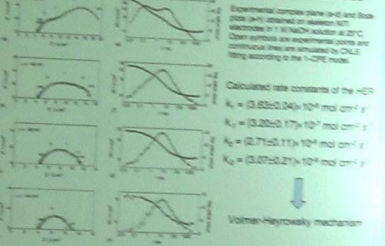
Steady state polarization curves
 Electrochemical measurements were performed using a VoltLab 10 potentiostat. Steady state polarization curves were registered potentiostatically in 1 mol/L NaOH (Merck, pur) with a scan rate of 1 mV/s. Before each measurement the working electrode (3 x 1 cm) is immersed for 300 s at -1.8 VSCE. The electrochemical activity of the electrodes was evaluated from the kinetic parameters derived from the linear part of the Tafel vs temperature dependence of the kinetic parameters and the activation energy for the HER was also determined.



Dependence of Tafel slope on NiTi electrodes in 1 mol/L NaOH, before and after the Tafel zone from which the kinetic parameters were determined.

Electrochemical Impedance Spectroscopy

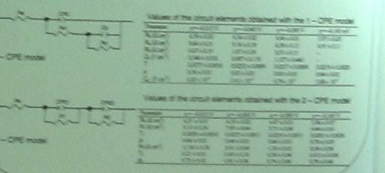
Impedance spectra were recorded in the frequency range 0 kHz to 10 MHz using a frequency response analyzer based on an AT-MIO 1675 National Instruments data acquisition board connected to an analogue P52 potentiostat. Measurements were conducted in potentiostatic mode at four different electrode potentials corresponding to moderate HER overpotentials (-0.215, -0.44, -0.595 and -0.745 V). The experimental data were fitted to the equivalent electrical circuit by a CHLS Levenberg-Marquardt procedure using the ZView-Software Associates Inc. software.



Experimental complex plane (a) and Bode plots (b) obtained on Raney NiTi electrodes in 1 M NaOH solution at 25°C. The linear fit to the experimental data and the equivalent circuit are shown in (c) and (d) respectively according to the 1-CPE model.

Calculated rate constants of the HER
 $k_1 = (3.83 \pm 0.04) \times 10^{-4} \text{ mol cm}^{-2} \text{ s}^{-1}$
 $k_2 = (3.20 \pm 0.17) \times 10^{-4} \text{ mol cm}^{-2} \text{ s}^{-1}$
 $k_3 = (2.71 \pm 0.11) \times 10^{-4} \text{ mol cm}^{-2} \text{ s}^{-1}$
 $k_4 = (3.07 \pm 0.21) \times 10^{-4} \text{ mol cm}^{-2} \text{ s}^{-1}$

Volmer-Hayrovsky mechanism



Conclusions
 • It is observed, the Raney Ni electrode with a higher real surface area should have a better activity for the HER, in fact the Raney NiTi electrodes show a much higher activity for the HER, which can be related to the catalytic effect of Ti.
 • The addition of Ti significantly increases the real exchange current density and confers an enhanced activity, despite the large value of the Tafel slope. Also, it reduces the electrochemical activation energy for the HER.
 • Electrochemical impedance studies revealed that the 1-CPE model describes the behavior of Raney NiTi electrodes. The impedance spectra indicated the presence of two potential-dependent semicircles of reduced HER overpotentials. Both semicircles were related to the HER kinetics. The determined double layer capacities slightly decrease with the overpotentials, indicating that a small fraction of the real surface is blocked by gas bubbles.
 • The rate constants determined by nonlinear approximation indicate that the HER takes place through a Volmer-Hayrovsky mechanism.
 Acknowledgment: The authors thank Romanian Ministry of Education and Research for financial support offered through CEEX (module 1) nr. 758/2008.



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