Computational material research and bioinformatics study at SU

E. Khosravi

October 31, 2008

Outline

1. Introduction to Southern LONI people
2. Thermal barrier coating research
3. gK and UL20 virus protein structure prediction homologe analysis
4. Simulation of raising bubble(Fluid dynamics)

Southern's LONI people

SU Faculty:

- **Habib Mohamadian**
- **Michael Stubblefield**
- **Dwayne Jerro**
- **Ebrahim Khosravi**
- **Edgar Blevins**
- **Michael Ralph**

Computational Scientist:

- **Shizhong Yang**

Graduate Fellow:

- **Frank DeTiege**
- **Christopher Clayton**

Collaborators: SU CEES Center

New LONI faculty at SU

1. Dr. Rachel E. Vincent-Finley (Computer Science)

   Numerical analysis, Molecular dynamics with reduced coordinate space

2. Wei Zhang ? (Mechanical Engineering)

   Composite material fabrication and analysis

New Highly Reflective Thermal Barrier Coatings

Dr. Shengming Guo(LSU ME)

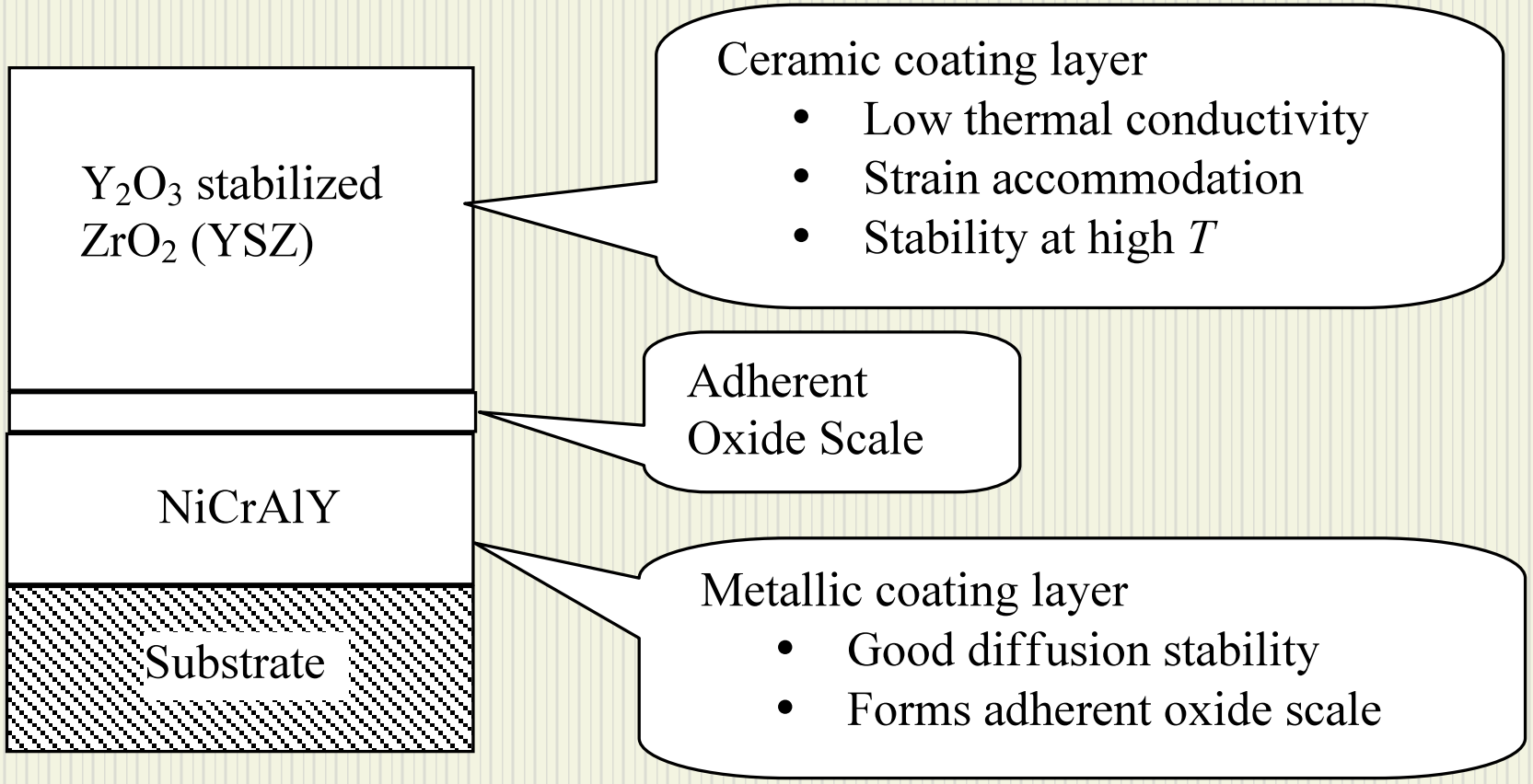
Dr. E. Khosravi(LONI/SU CMPS)

Dr. Shizhong Yang(LONI/SU CMPS)

Motivation:

- **TBCs are used in the hot section of rocket and jet engines to safeguard them under extreme working temperatures, ~1600°C.**
- **Regular YSZ, is translucent in both visible and infrared bands.**

Goal: develop high R TBC



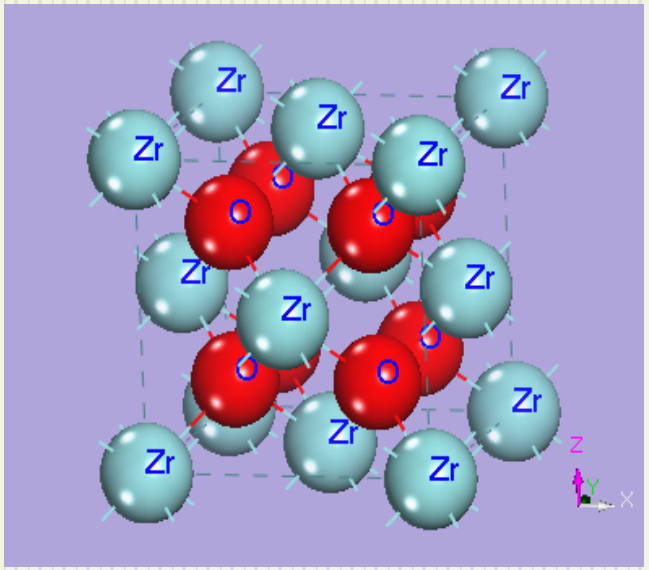
Schematic of a TBC system

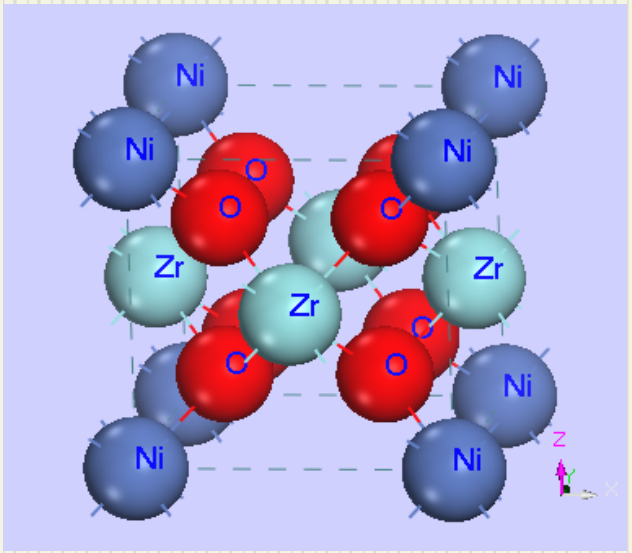
Method I: The TBC with Multilayer of Alternating Reflectance

- Ab initio Molecular Dynamics simulations was used to calculate ZrO2/Al2O3 interface under different T and P. VASP package was used.

- Optical properties will be calculated to guide the experimental study.

Method II: Ni doped ZrO2

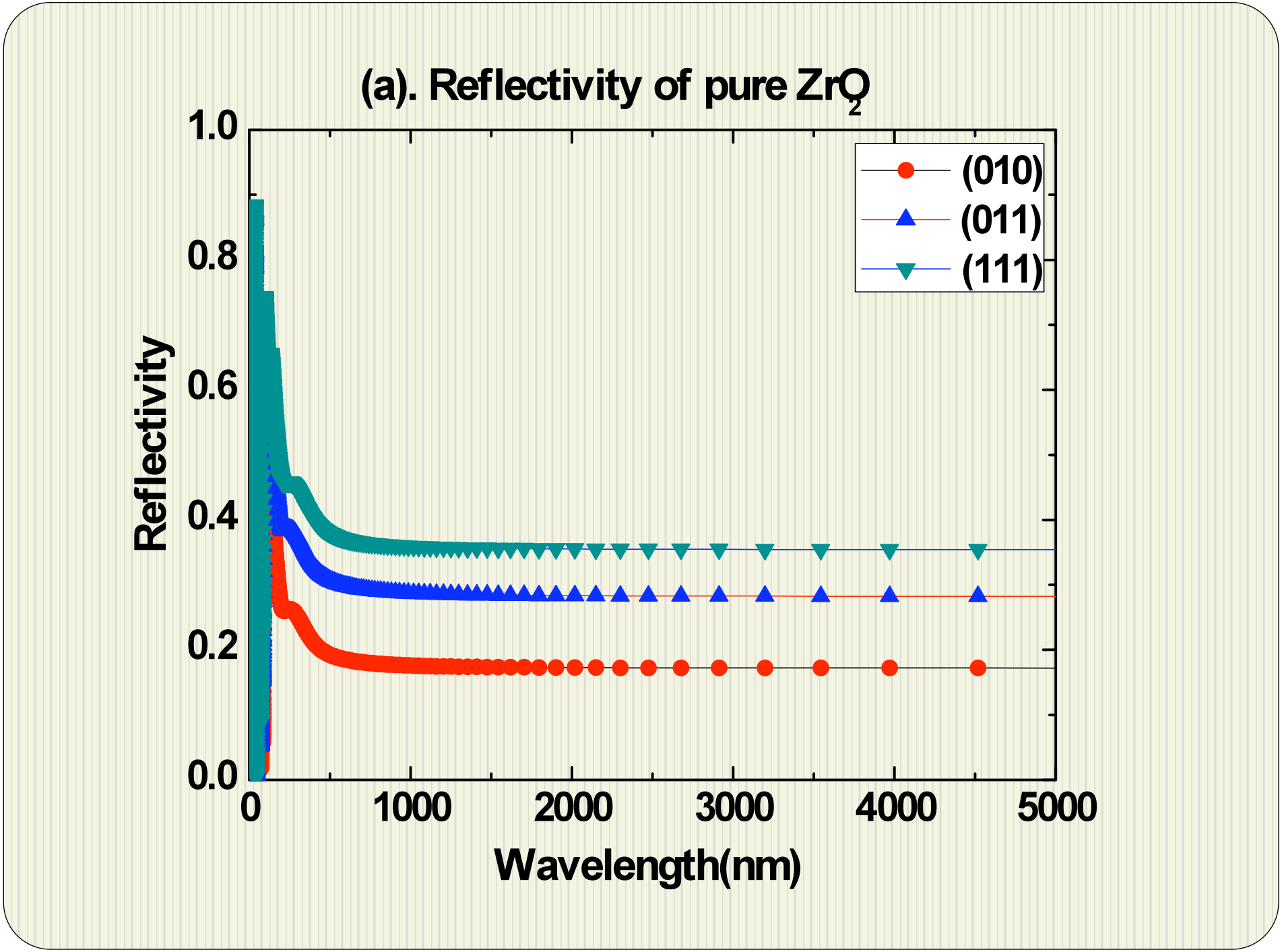


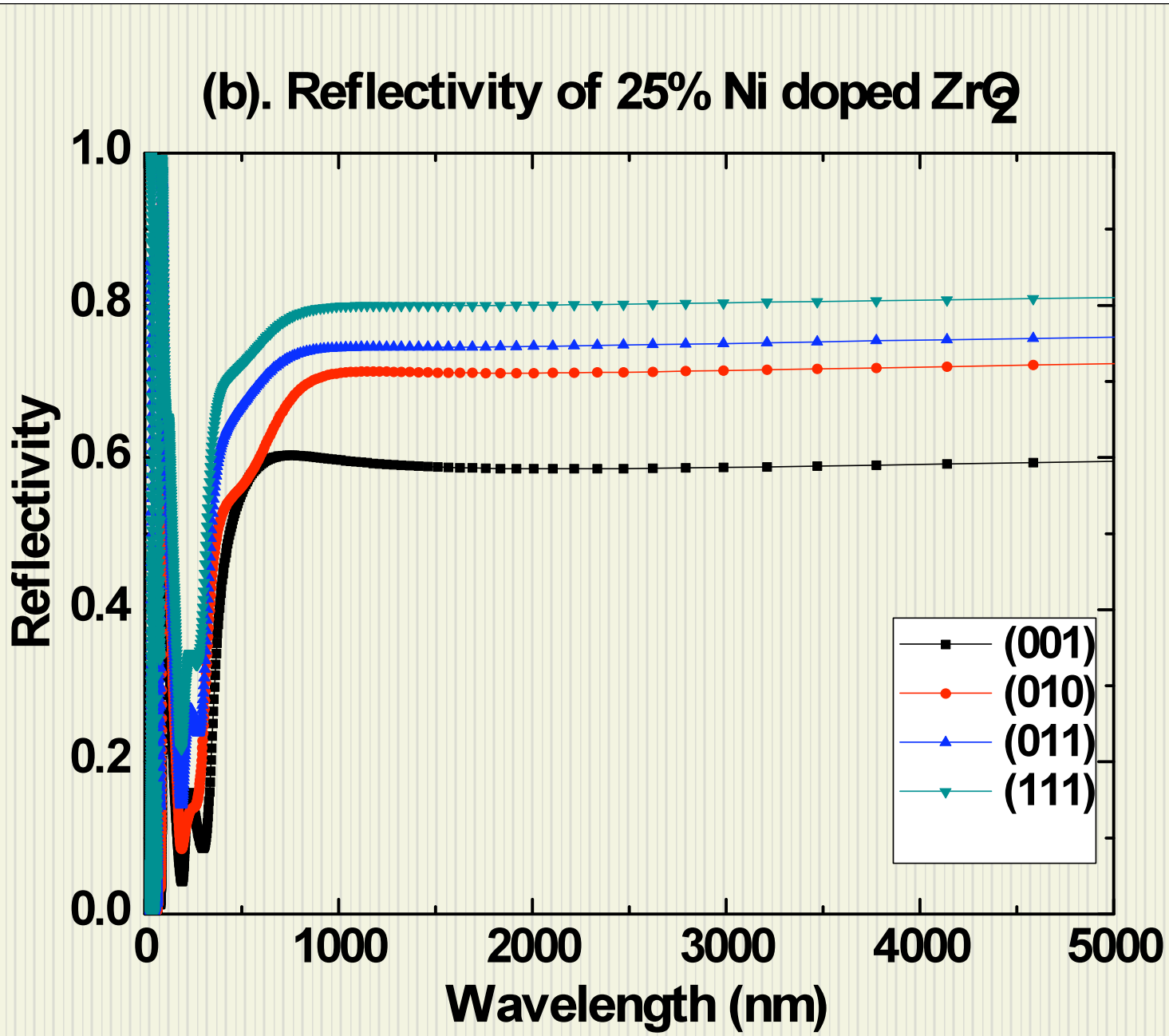


25% Ni doped ZrO2 models

Properties studied:

- Elastic constants
- Bader charge
- Density of states
- Bonding
- Stability
- Optical property


(a). Reflectivity of pure ZrO2
Reflectivity
Wavelength(nm)
1.0
0.8
0.6
0.4
0.2
0.0
0
1000
2000
3000
4000
5000
(010)
(011)
(111)

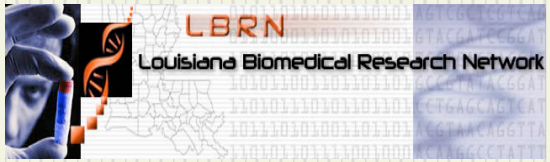

(b). Reflectivity of 25% Ni doped ZrO2
Reflectivity
1.0
0.8
0.6
0.4
0.2
0.0
0
1000
2000
3000
4000
5000
Wavelength (nm)
(001)
(010)
(011)
(111)

Prediction of Conserved and Divergent Secondary Structure Features of Virus UL20p and gK Proteins

Dr. Shuji Bai; Dr. Ebrahim Khosravi

Dr. K. Gus Kousoulas; Dr. Marcia Newcomer

Dr. Shizhong Yang; Mr. Christopher Clayton



Motivation:

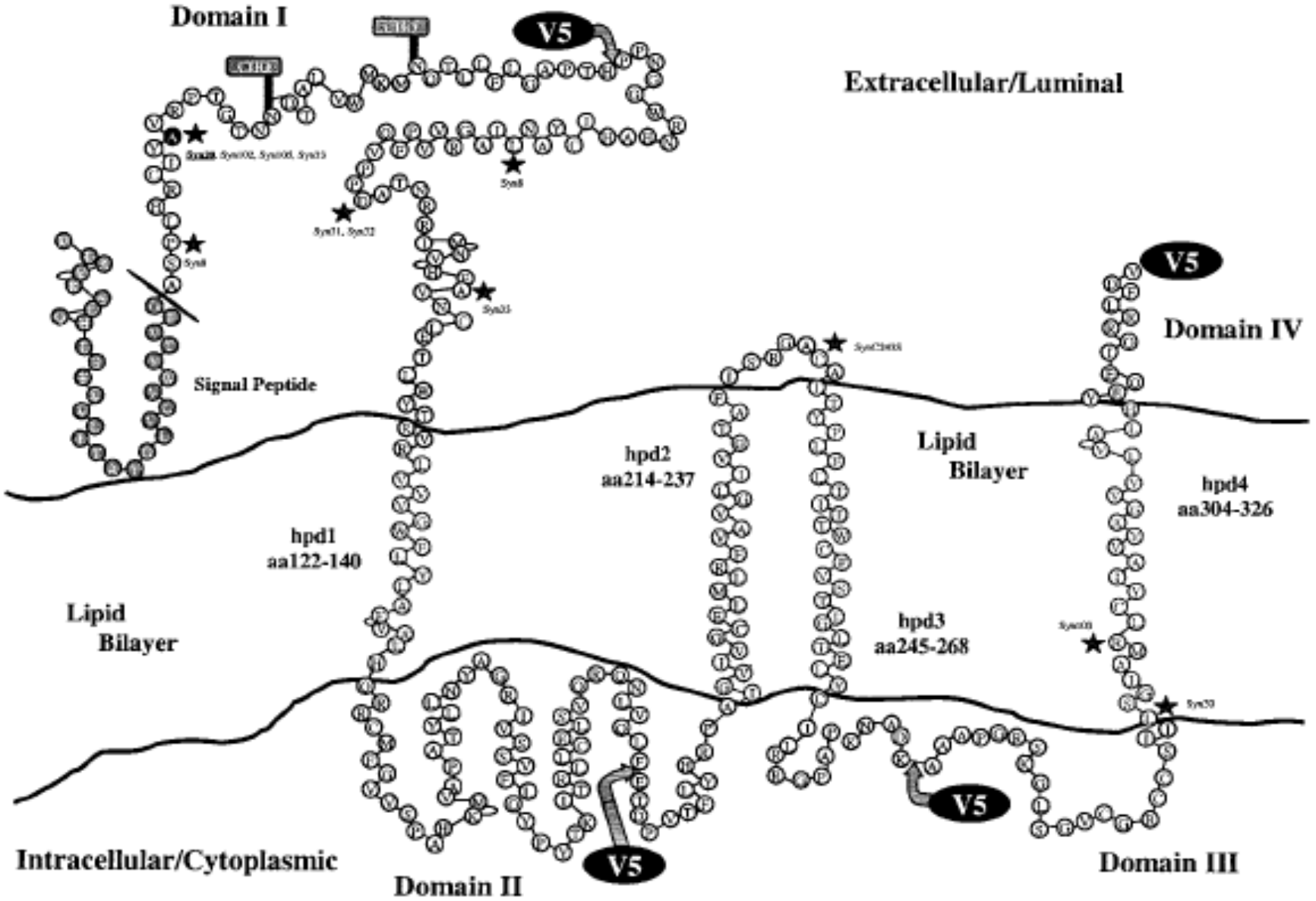
- Understanding the secondary structures of trans-membrane virus gK and UL20 could greatly facilitate predicting functional domains of each protein that may be involved in multiple functions through the virus lifecycle

Methods used:

- Hiden Markov Model
- Neuro Network

Works done:

- **1. Tested all the available codes and compared gK results with experimental data.**
- **2 . Hiden Markov is better than Neuro Network method in gK virus structure prediction.**
- **3. Successfully predicted signal peptides for both gK and UL20.**



Experimental gK membrane topology
J. Virology, 77, 499 (2003)

Future works:

- gK and UL20 homolog alignment and functional analysis
- Molecular dynamics study the interaction between gK and UL20.

Simulation of Rising Bubble

Dr. H. Dwayne Jerro

Dr. Samuel Ibekwe

Frank DeTiege: LONI graduate fellow

Motivation:

- **Fluid Dynamics: The ultimate goal of this research is to safely enhance the heat transfer between a nuclear reactor and its coolant without raising the reactor's operation temperature by boiling through microstructures.**

Research Focus:

- **This research is focused on a three dimensional simulation of vapor bubbles being generating and rising in the presence of microstructures.**

Solution Setup

- Gambit Specifications
  - Water Column 0.5m by 1.5m
  - Mesh faces: 14700 control volumes
  - **FLUENT® was used.**
- FLUENT Universal Procedure – Part 1
  - Unsteady Solver
  - Multiphase Model
    - Volume of Fluid with Implicit Body Force
  - Definition surface tension between phases
  - Operating Conditions
    - Gravity
    - Specified Operating Density
    - Reference Pressure
  - Boundary Conditions
    - Top Wall – Pressure Outlet
    - Right and Bottom Wall – Wall
    - Left wall - Symmetry
  - Solution
    - Body Force Weighted for Pressure
  - Residual

Solution Setup Continued

- FLUENT Universal Procedure – Part 1
  - Unsteady Solver
  - Multiphase Model
    - Volume of Fluid with Implicit Body Force
  - Definition surface tension between phases
  - Operating Conditions
    - Gravity
    - Specified Operating Density
    - Reference Pressure
  - Boundary Conditions
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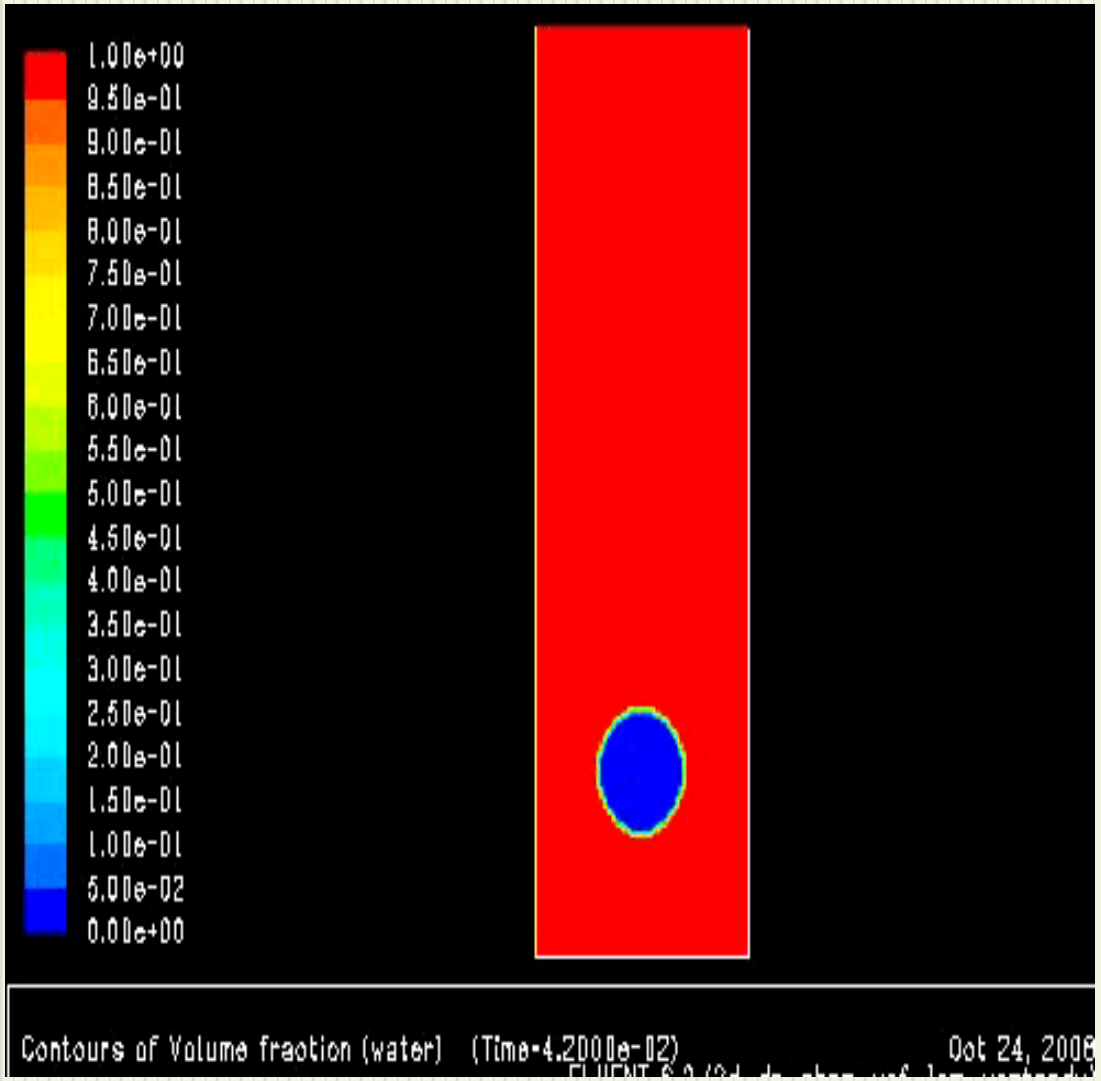
  - Solution
    - Body Force Weighted for Pressure
  - Residual

Solution Setup Continued

- FLUENT Process Procedure – Part 2
  - Initialization
  - Iterate
    - Time Step Size = 0.001s
    - Number of Time Steps = 1000
    - Max Iterations per Time Step = 100
  - Region
    - Circle with a radius of 0.1m
    - Reference location (X,Y): 0.25m, 0.3m
  - Patch
  - Solution Animation
  - Iterate

Results

- Simulated rising bubble by use of the “patch” built in function.

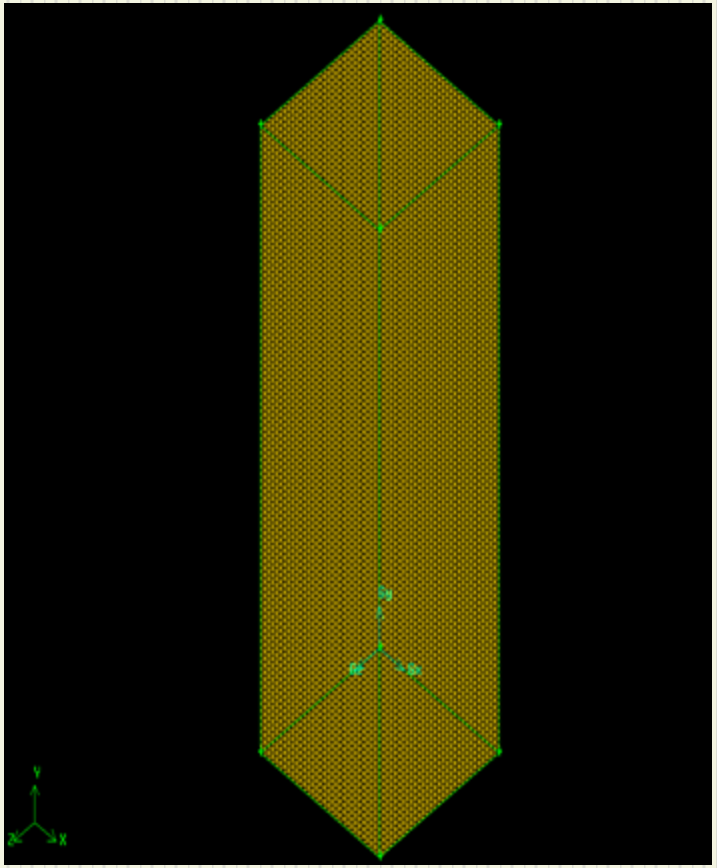


Works finished:

- **A two-dimensional simulation of an air bubble rising in a water column has been successfully created by using a built in function called “patch”.**

Future Plans

- **Three dimensional simulation of bubble column**



Thank you for coming.

- **Questions?**