Teaching Computation & Modeling in Materials Engineering

Shahriar Anwar

School of Materials
Arizona State University
Tempe, AZ 85287

MSE 315 – Mathematical & Computational Materials Engineering (3 Credits, required)

- **Objectives**
  Introduce broad array of computational and mathematical techniques integrated with materials science and engineering issues.

- **Catalog Description**
  Introduction to programming, modeling and mathematical techniques.

- **Prerequisites**
  Introduction to Materials Science and Engineering (MSE 250).

- **Textbooks**
  Fortran 90 by Nyhoff & Leestma and Advanced Numerical Methods by S. Rao.

- **Laboratory**
  Lecture twice a week integrated with lab activity.

Topics

- UNIX, Fortran, and Matlab
- ODE, PDE, system of equations, stochastic methods
- Lab View: Electrical resistivity vs. temperature
- **Finite element modeling: crack growth & precipitation hardening**
- **Cast Metallic Alloys: Microstructure characterization and modeling of thermal and mechanical properties by Object Oriented Finite Element (OOF) Analysis**
- **Bimetallic Strips: Thermal expansion behavior**
- Design of Experiments

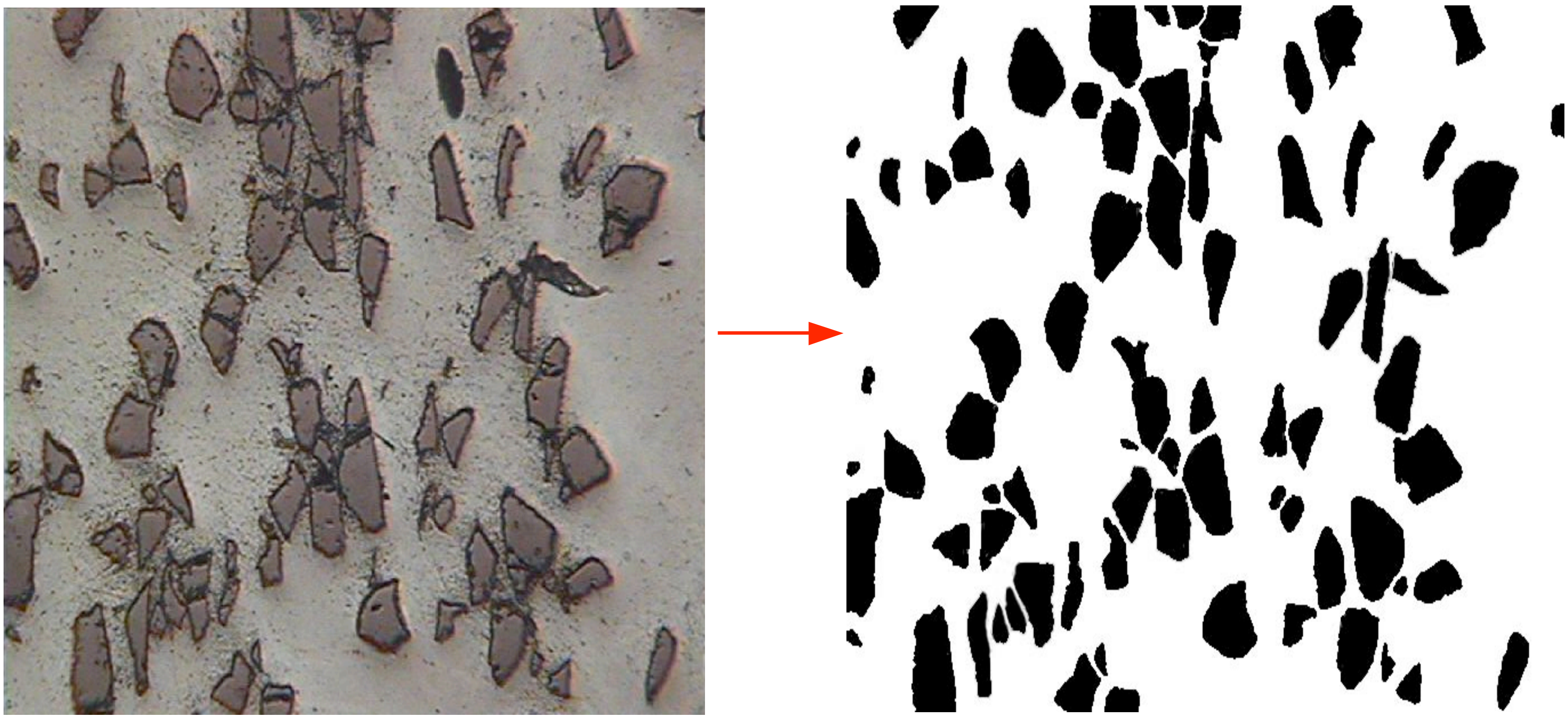
Outcomes

- Understand the basics of the UNIX operating system.
- Understand the fundamentals of programming style including program compiling, data structures, function calls, and subroutines and apply these to solving materials engineering problems.
- **Can acquire and analyze optical and SEM images of microstructures and relate them to their phase diagrams.**
- **Learn the fundamentals of finite element analysis and apply them to model materials and test their properties.**
- Learn the principles of superconductivity and to measure their properties.
- Learn to solve ODE and PDE numerically and .solve diffusion, heat conduction, and spectral problems.
- Learn how to do design of experiments and apply this knowledge to improve materials properties.

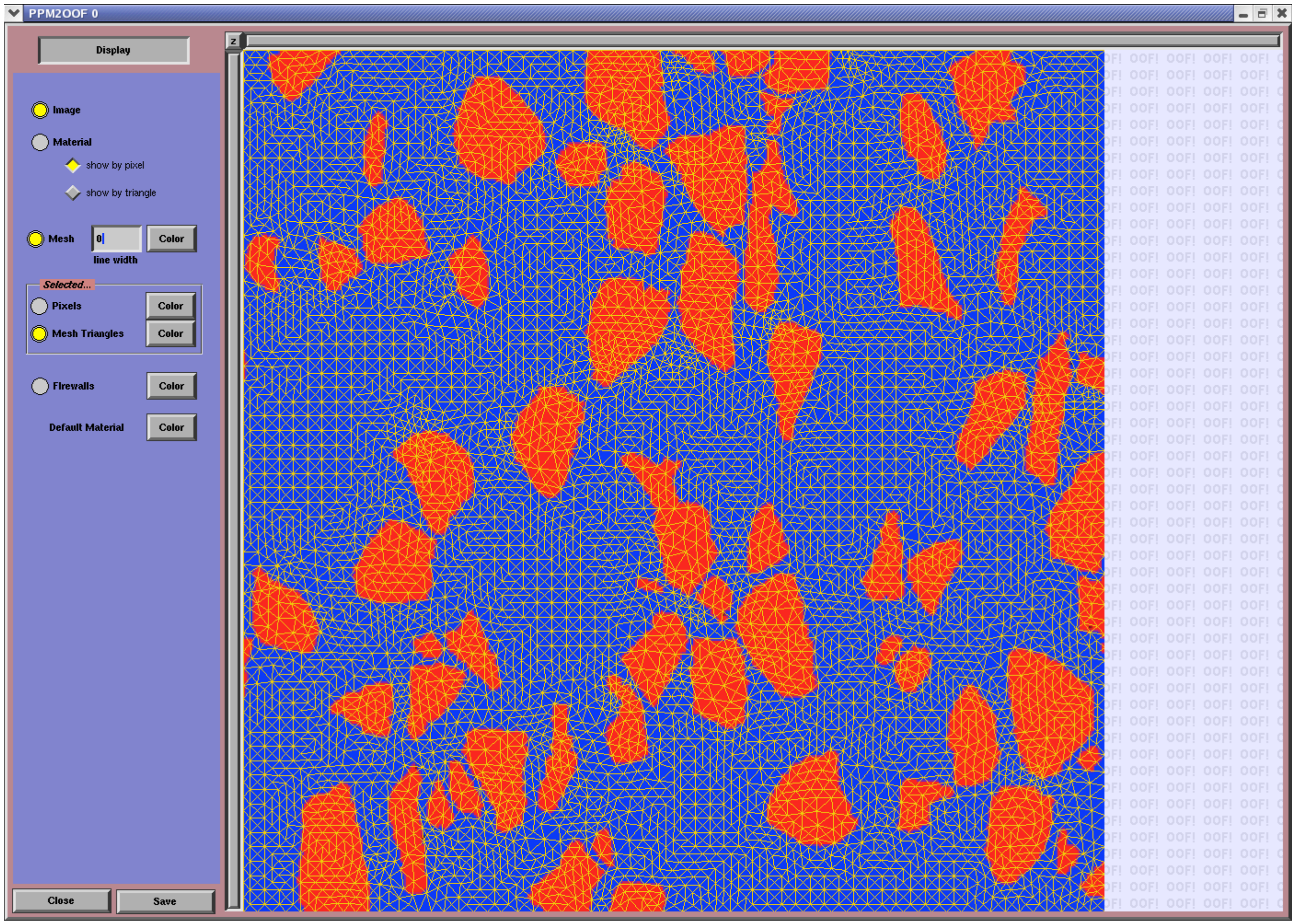
Virtual Experiments

- Thermal properties of SiC particle reinforced Al matrix composites
- Thermal Expansion of a Bimetallic strip
- Mechanical Properties of Eutectic Alloys (Pb-Sn solder)
- Stress concentrator vs. crack length and radius

Segmentation of Al/SiC Micrograph



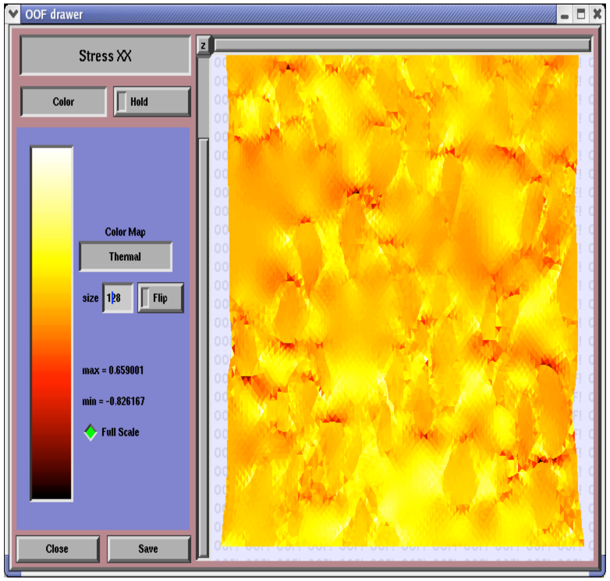
Simulation of Al/SiC



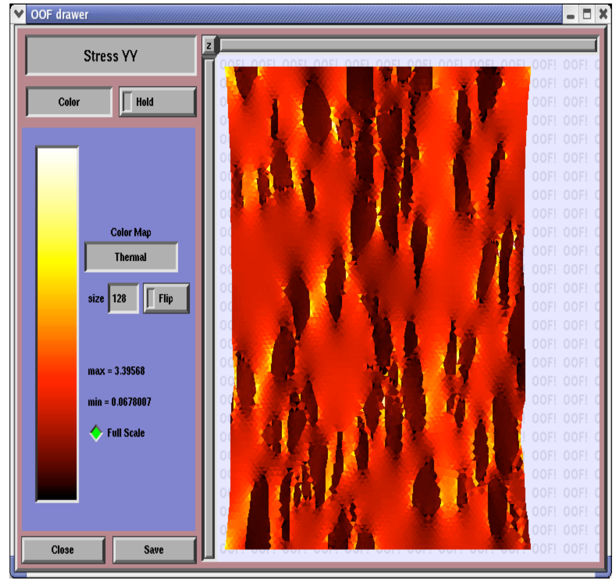
Final mesh (E refined for two additional iterations)

→ 7,416 nodes and 14,584 elements (started with 960 nodes and 1,800 elements)

Simulation of Al/SiC – Axial Loading



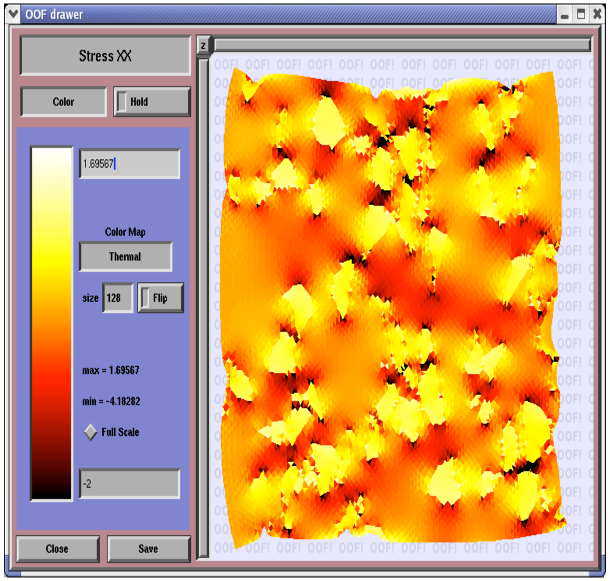
σ_{xx}



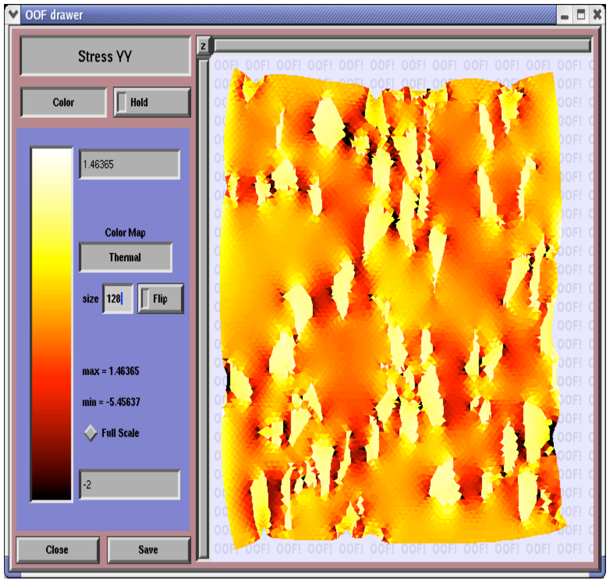
σ_{yy}

- Apply strain in y-direction, (ε_{yy} = 1%)
- Analyze stress in x-direction (σ_{xx}) and y-direction (σ_{yy})
- Note anisotropy of microstructure and effect on local stress distribution

Simulation of Al/SiC – Thermal Expansion



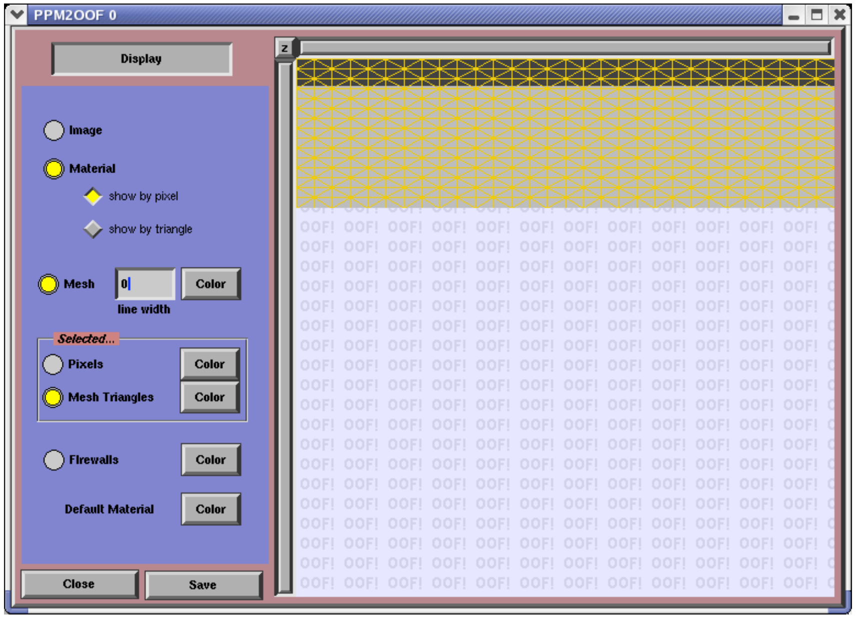
σ_{xx}



σ_{yy}

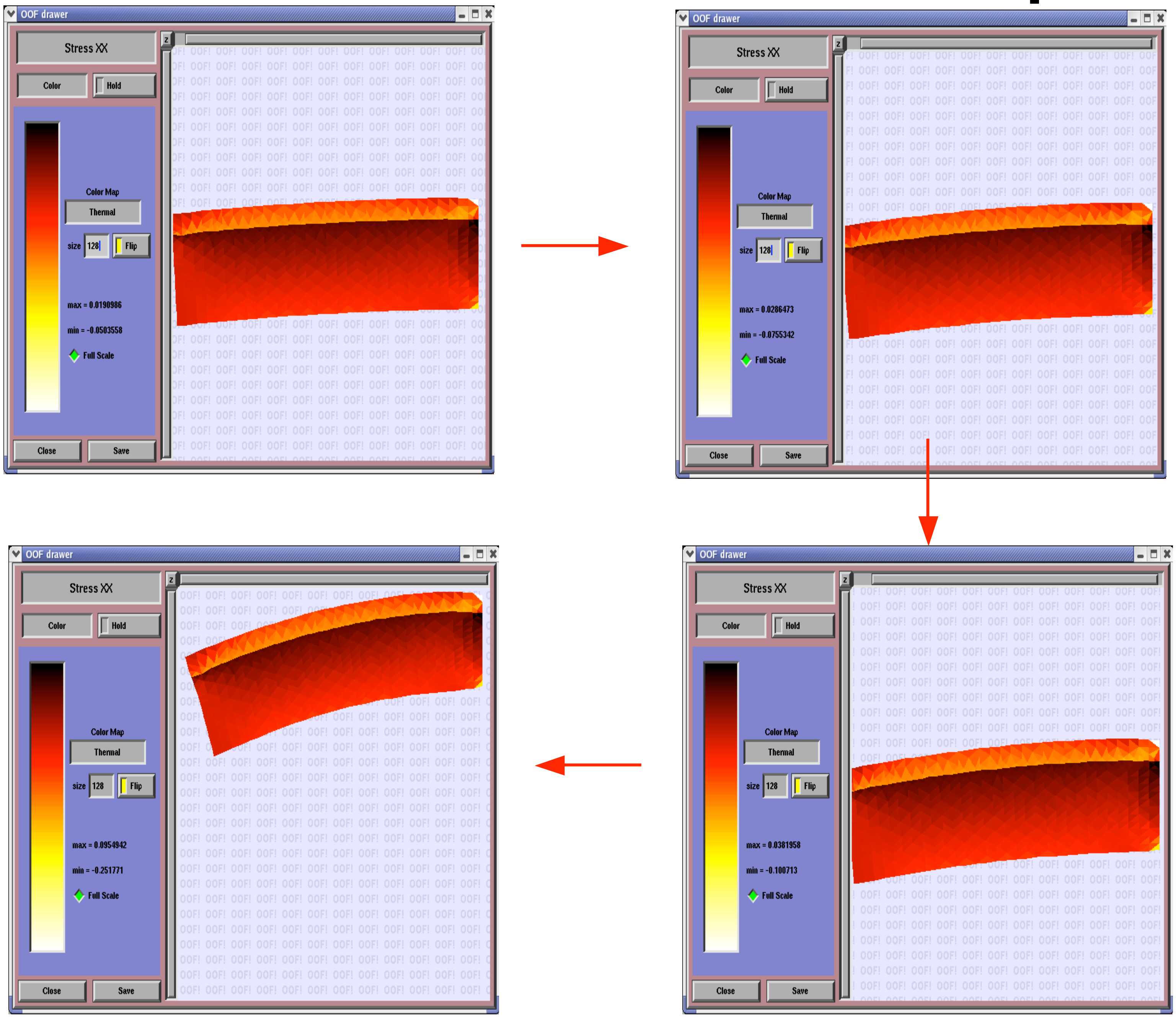
- Thermal stress on unconstrained composite
- Raise temperature incrementally and equilibrate
- Observe σ_{xx} and σ_{yy}
- Note anisotropy in thermal expansion. Sample has been expanded 47% in x-direction and 58% in y-direction

Simulation of Thermal Expansion of Bimetallic Strip



• Students were also asked to calculate radius of curvature of bimetallic strip using analytical expressions.

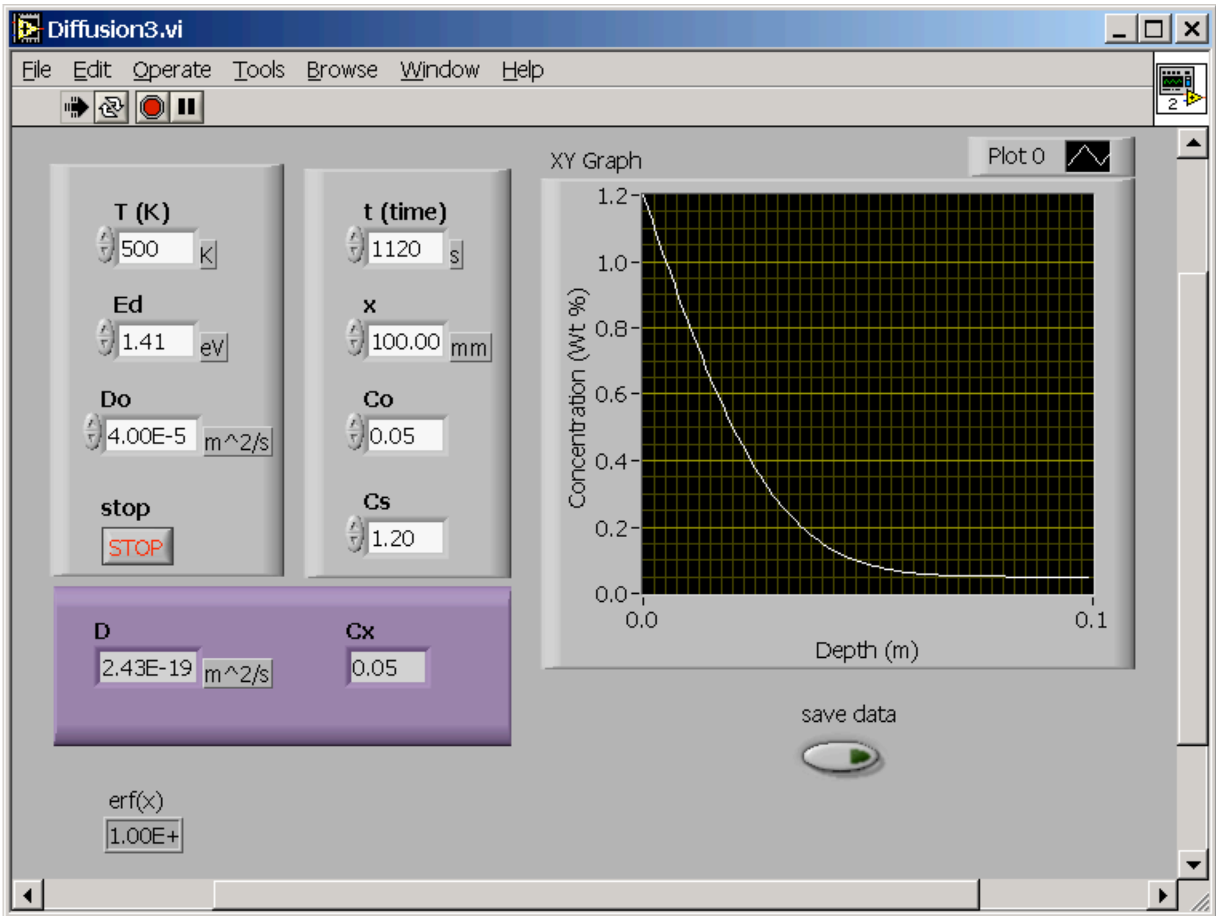
Simulation of Bimetallic Strip



Casting Procedure for Pb-Sn Alloy

- Weigh Sn pellets in a crucible and heat to a melt
- Add amount of Pb to achieve desired composition and heat at 350 °C for 30 minutes
- Pour Pb-Sn molten alloy into a steel mold designed for tensile testing
- Quench the mold in water and remove the sample
- Carry out tensile testing
- Observe cross sections of the broken samples under a microscope
- Obtain digital micrographs to be used in OOF
- Repeat to cast four different compositions of Pb-Sn

Diffusion Problem in LabView



Conclusions

- Microstructure-based modeling, using Object Oriented Finite Element Analysis, was incorporated in an undergraduate materials course
- Students conducted virtual experiments on thermal and mechanical behavior of SiC/Al composites, bimetallic strip, and Pb-Sn solder
- Quantitative student feedback indicated an increase in knowledge level and understanding of microstructure and its effect on mechanical properties

Acknowledgments

- The OOF team for the ongoing development of this application.

- Steve Langer for helping us implement OOF deployment at ASU.