Phase-field Method in Analysis of Nanocomposite Morphological Stability

Andrei Klishin[1], Peter Mayr[2], Michael J. Demkowicz[3]

[1] Massachusetts Institute of Technology, Physics Dept.
[2] Chemnitz University of Technology, Chair of Welding Technologies
[3] Massachusetts Institute Technology, Dept. of Material Science and Engineering

Sponsored by MIT-Germany program

COMSOL CONFERENCE BOSTON 2013

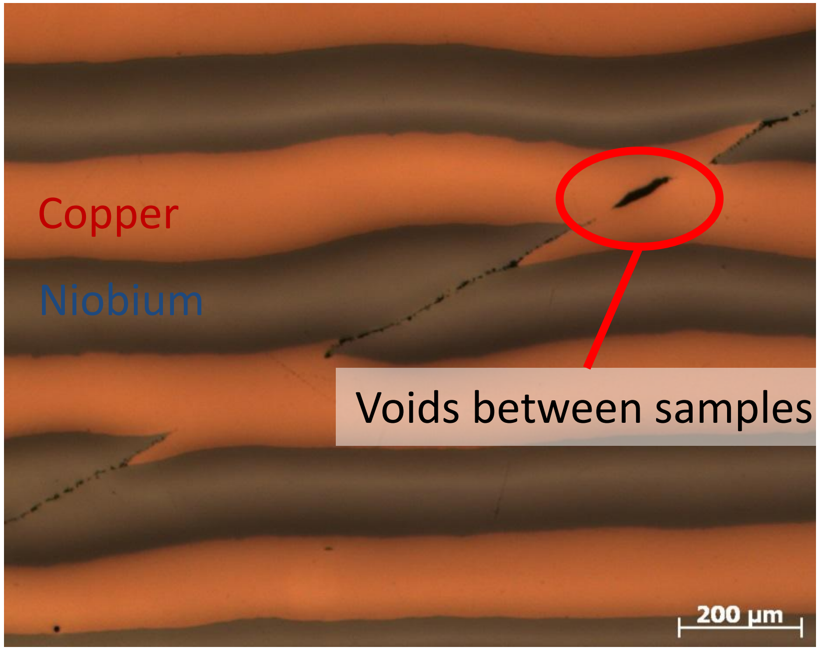
Massachusetts Institute of Technology

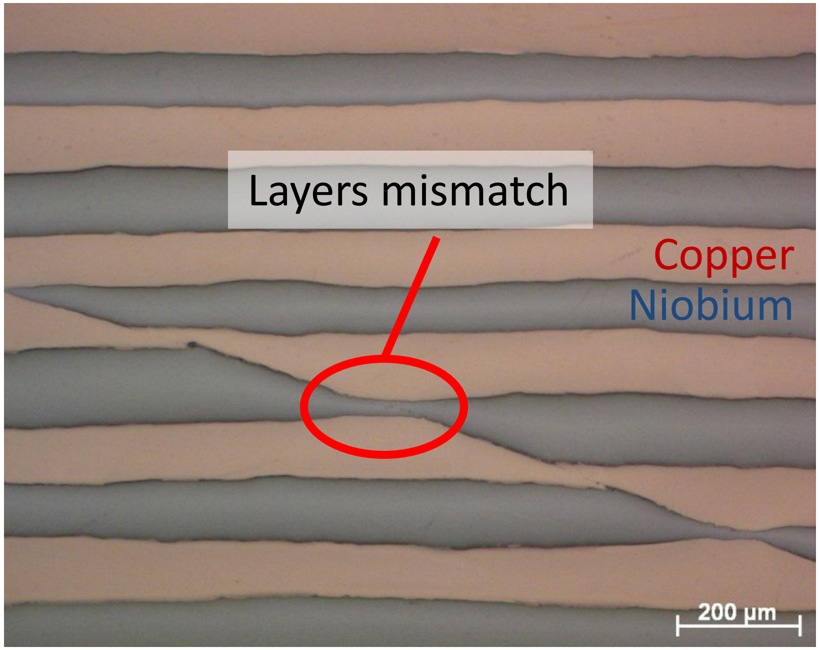
TECHNISCHE UNIVERSITÄT CHEMNITZ

Problem of joining defects

Joining method of choice: diffusion welding

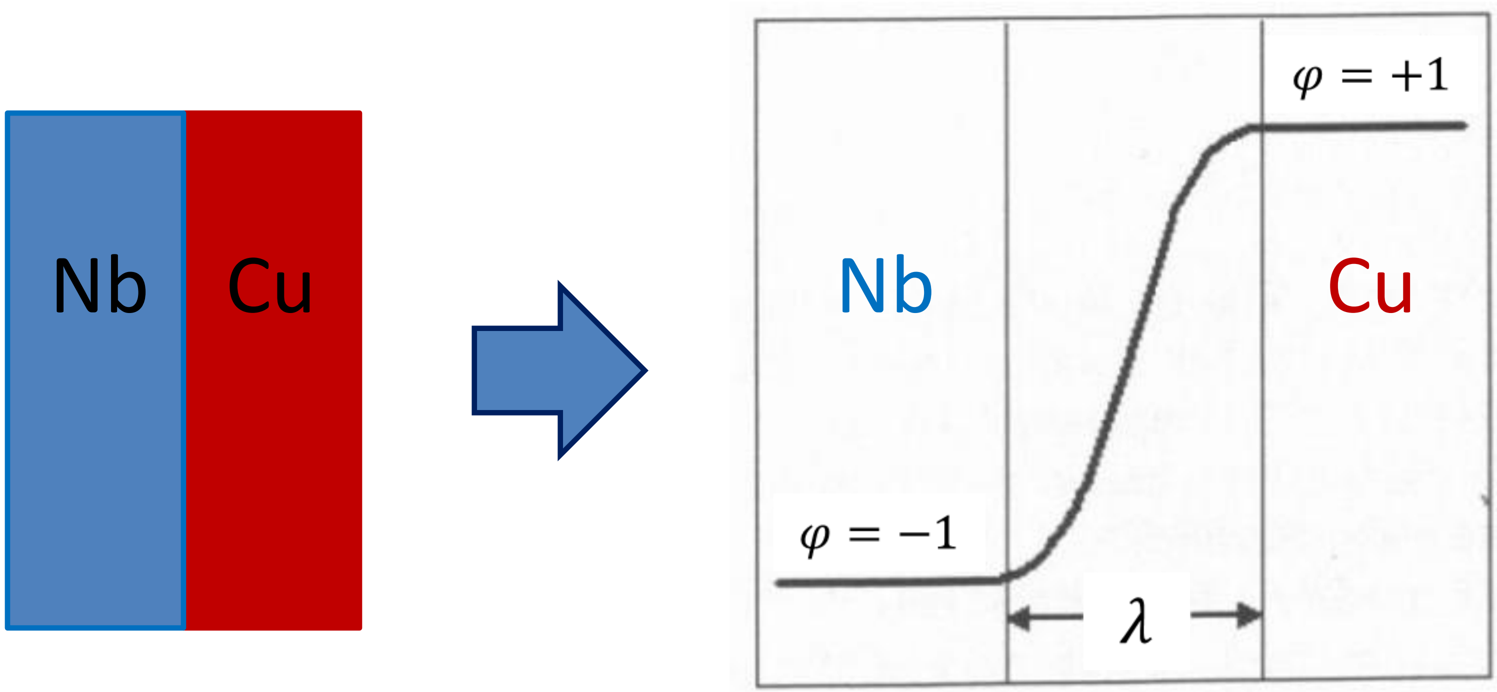
Question: are the welding defects stable under exposure to high temperature and pressure for extended periods of time?





Images courtesy of Stefan Habisch, Chemnitz University of Technology

Phase-field method equations

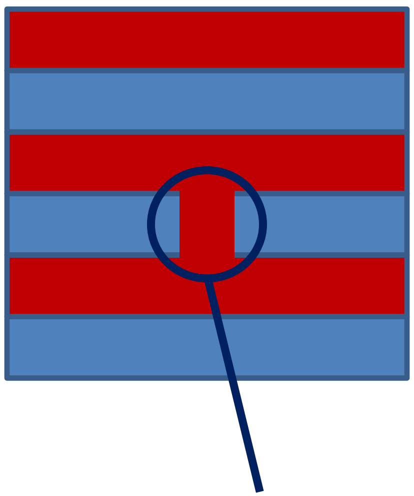


Cahn-Hilliard equation for phase separation:

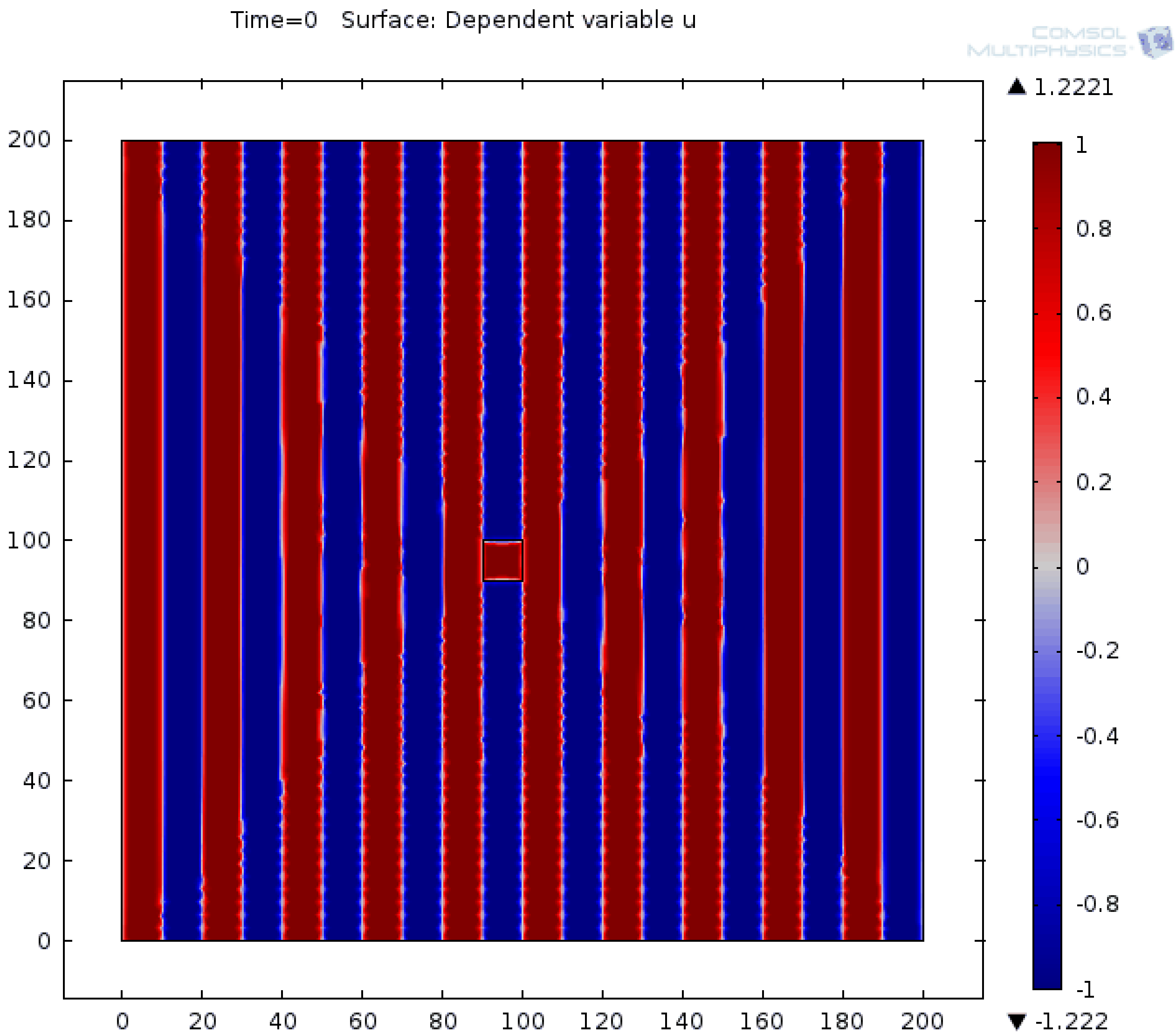
$$\frac{\partial \varphi(\vec{r}, t)}{\partial t} = M \nabla^2 \left(-W_0 \nabla^2 \varphi + H(\varphi^3 - \varphi) \right)$$

COMSOL: coefficient form set of two PDEs

2D pinched layer instability

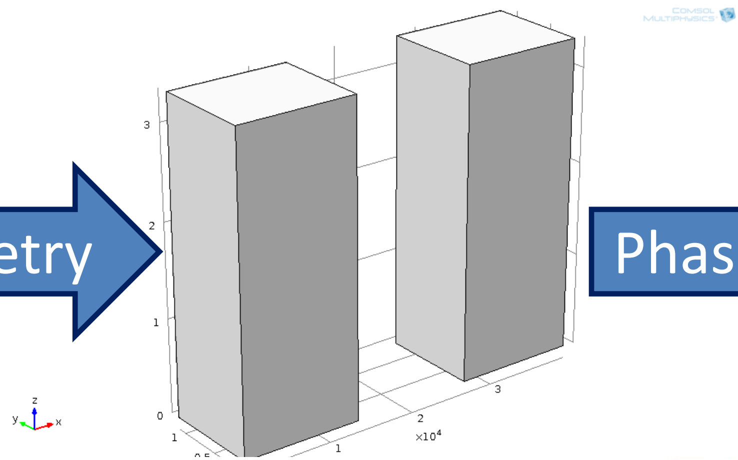


Cu pinchoff

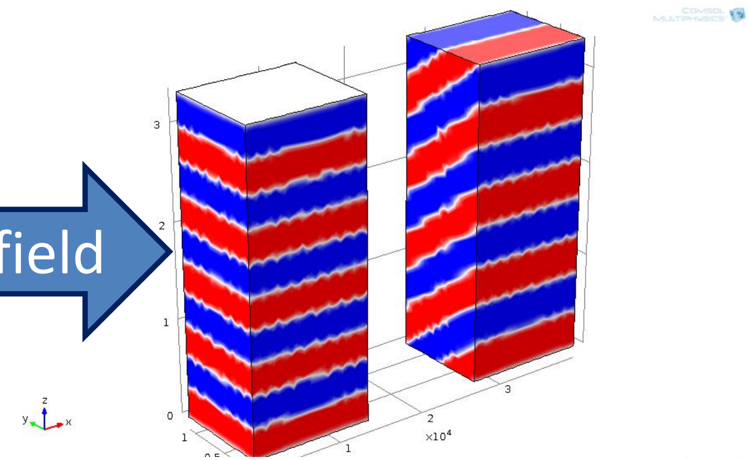


Model construction

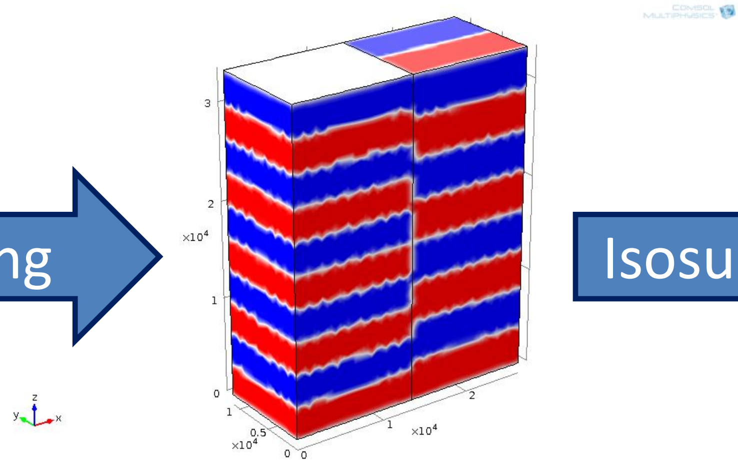
Geometry



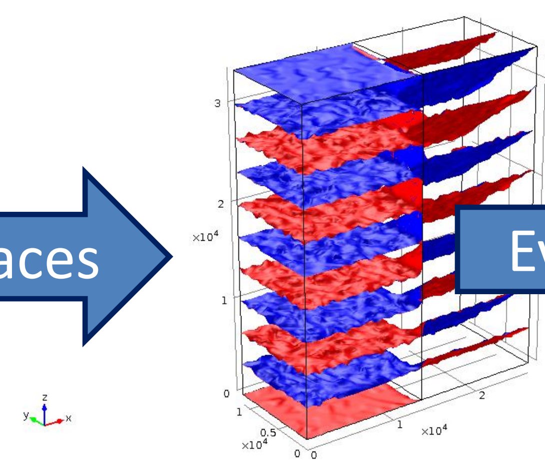
Phase field



Joining



Isosurfaces

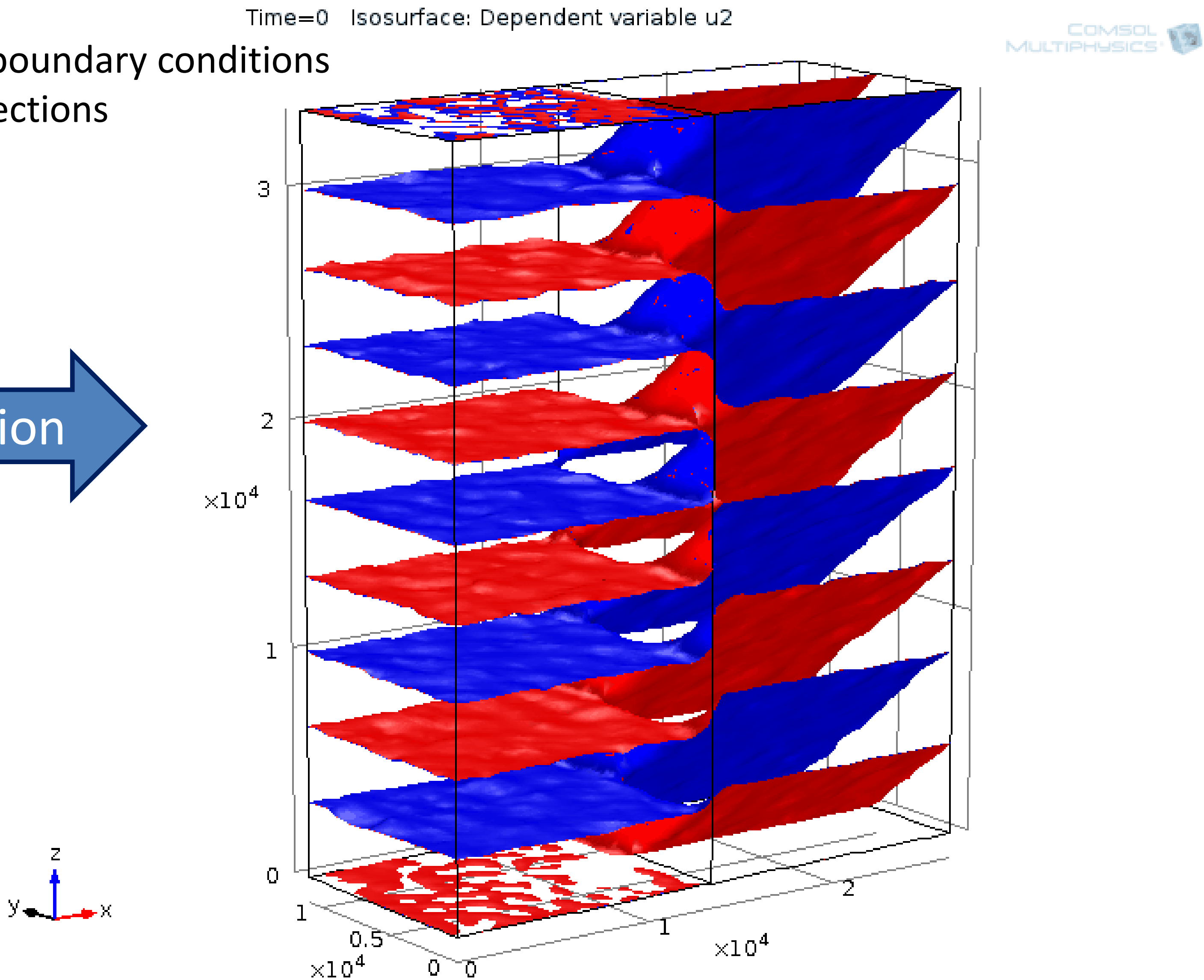


Evolution

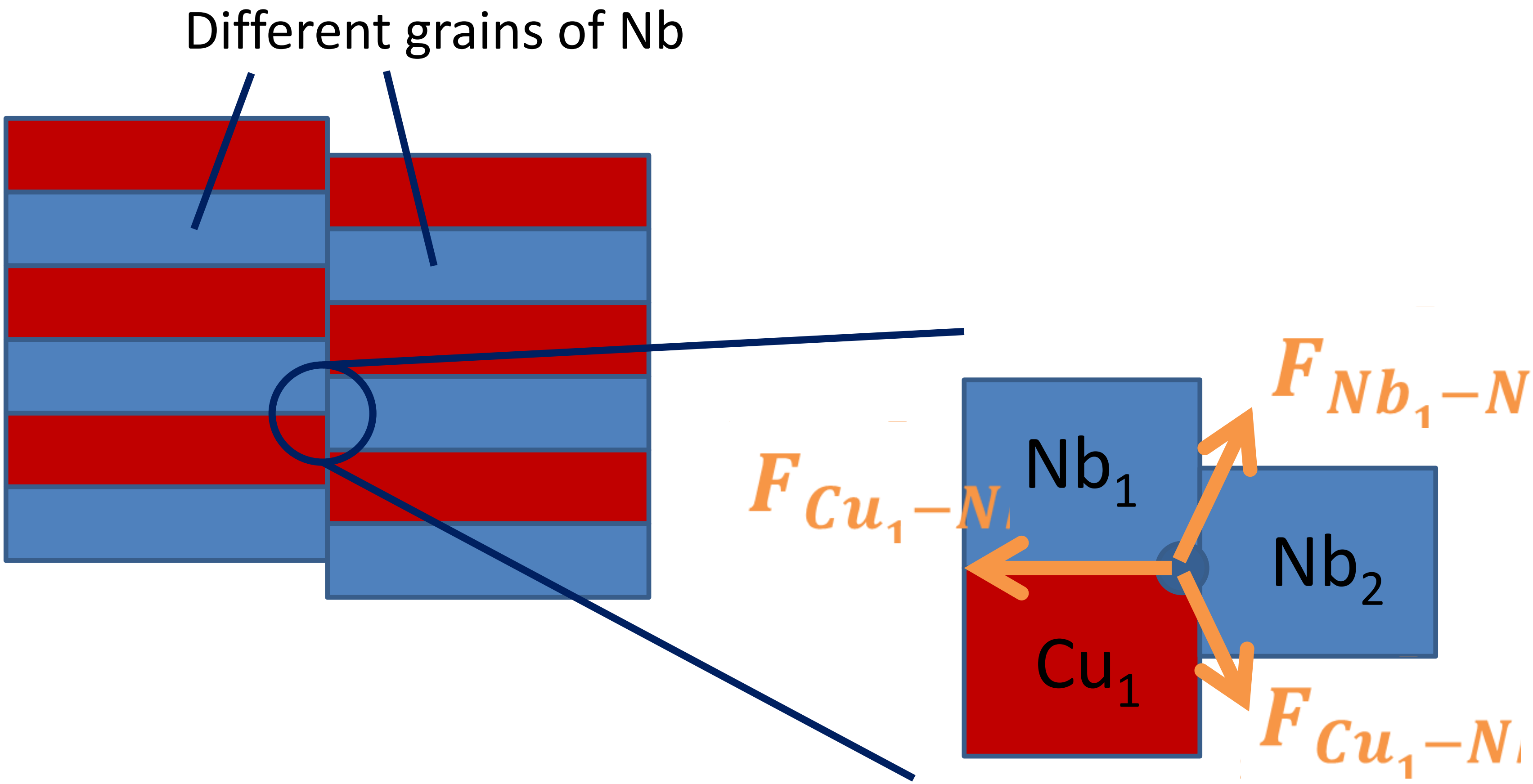
Twist defect

- Periodic boundary conditions in y, z directions

Evolution



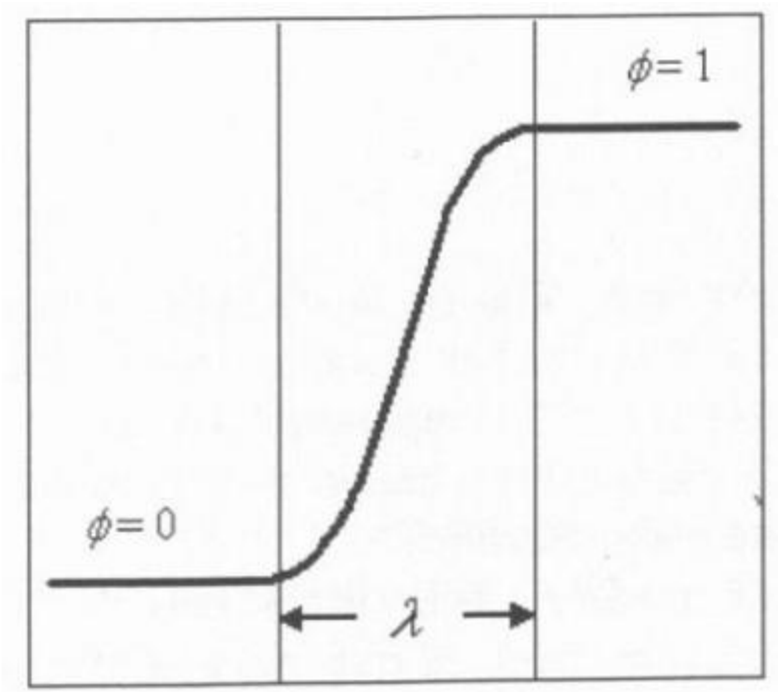
Inclusion of grain boundaries



Conclusions

- Phase-field model provides robust and accurate predictions of behavior of nanocomposite phase interfaces.
- Instability and indefinite collapse of layers is proven to be a typical feature of diffusion joints in 2D and 3D for single-phase-field model.
- It may be possible to hinder joining instabilities by incorporating the boundaries between the adjacent grains into the model

Phase-field method introduction



- Sharp interfaces are replaced with continuous phase-field with some normalization
- Free energy of the composite calculated in every point
- System tries to minimize free energy, which is manifested in the equations of motion
- Balance of Cu-Nb is maintained as a conserved order parameter

Free energy: $$F = \int [f(\varphi) + \frac{\alpha}{2}(\nabla\varphi)^2] d^3 r$$

Bulk energy Interface energy

Phase-field method equations

Cahn-Hilliard equation for phase separation:

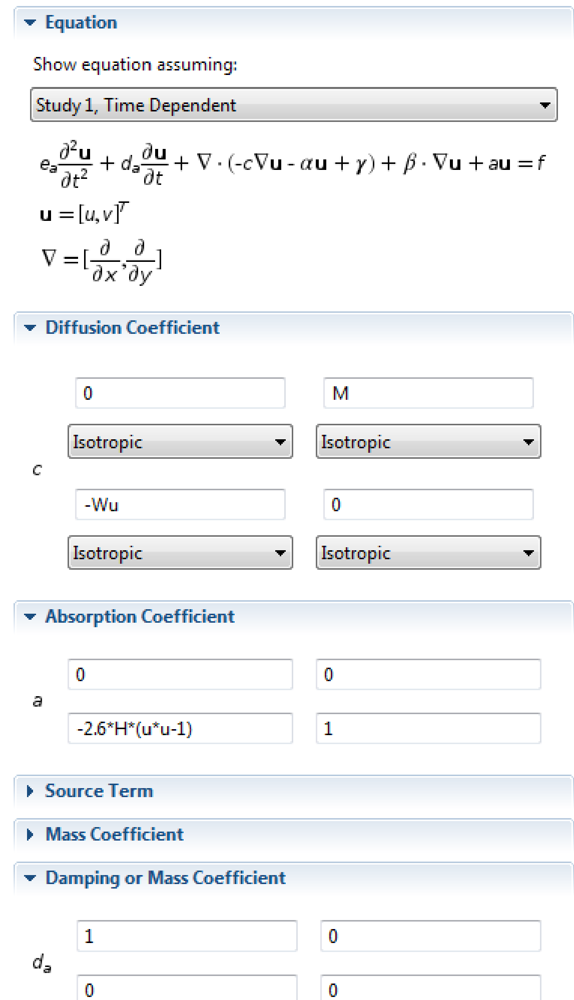
$$\frac{\partial \varphi(\vec{r},t)}{\partial t} = M\nabla^2\left(-W_0\nabla^2\varphi + \frac{\partial g}{\partial \varphi}\right)$$

Double-well potential:

$$g(\varphi) = H\left(\frac{\varphi^4}{4} - \frac{\varphi^2}{2}\right)$$

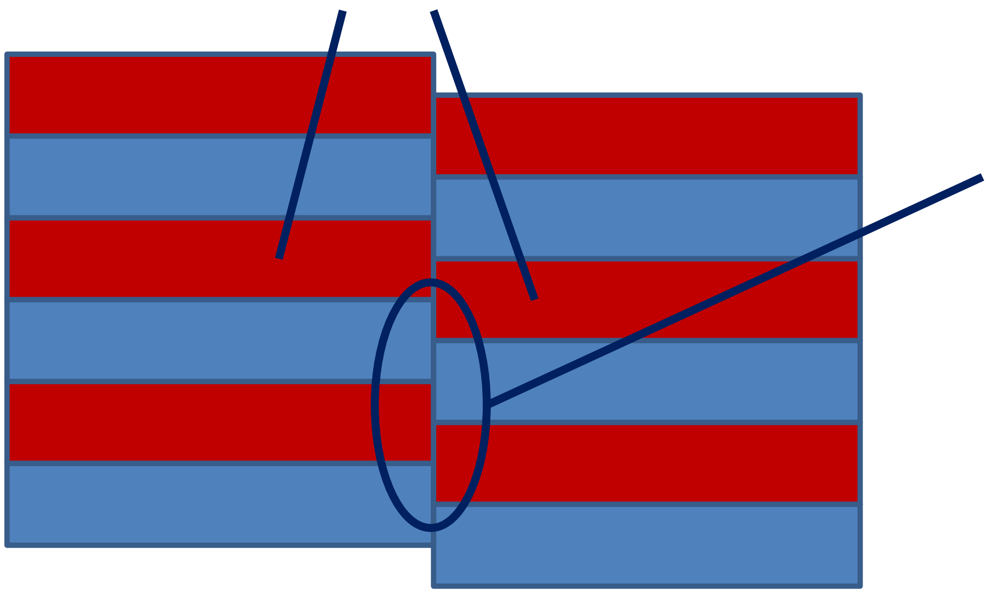
COMSOL implementation:
coefficient form set of PDEs (two PDEs for each conserved order parameter)

Allows easy expansion to include multiple order parameters



Inclusion of grain boundaries

Different grains of Cu



Can extra grain boundaries stabilize the joint?

Conserved order parameter

Cu-Nb field

two 2^{nd}-order PDEs
(Cahn-Hilliard eqn)

+

Non-conserved order parameter

Cu 1^{st} grain/Nb 1^{st} grain
Cu 2^{nd} grain/Nb 2^{nd} grain
...

one 2^{nd}-order PDE per used grain
(Allen-Cahn eqn)