PanROME

Development of A Practical Phase Field Tool

Kaisheng Wu, Shuanglin Chen, Fan Zhang and Y.A.Chang

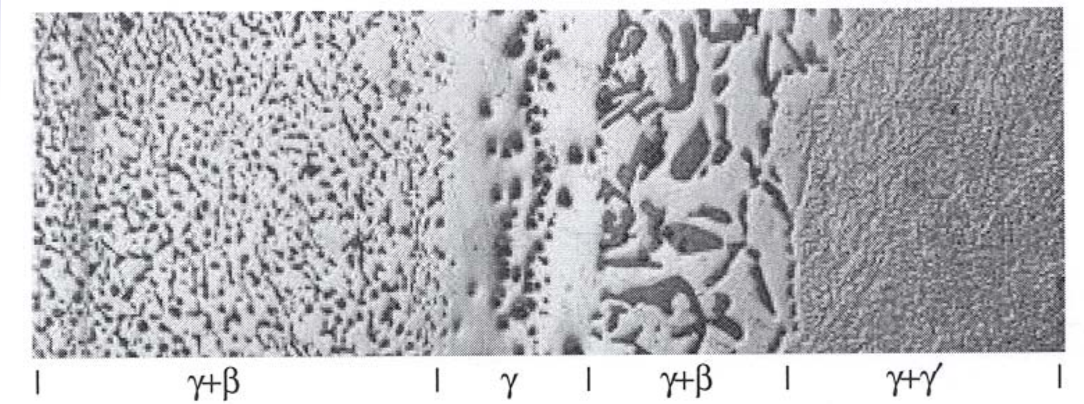
CompuTherm LLC, Madison, WI

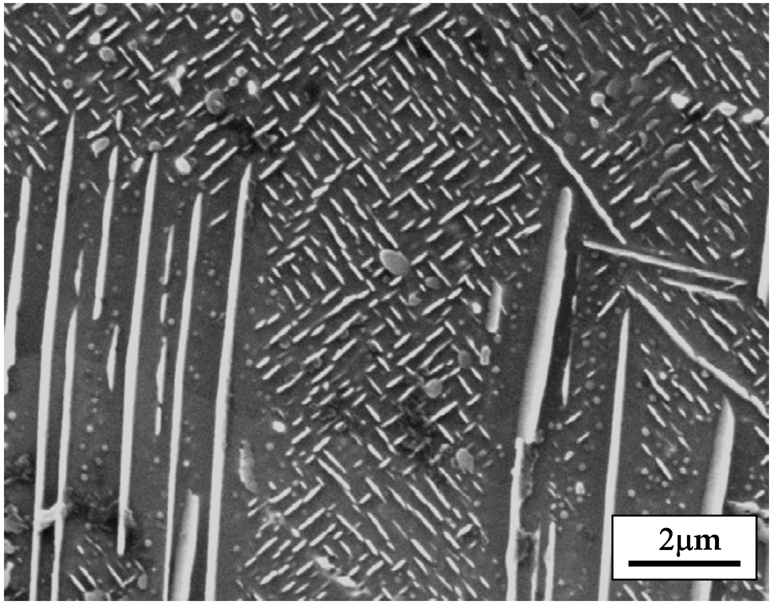
Ximiao Pan and Yunzhi Wang

The Ohio State University, Columbus, OH

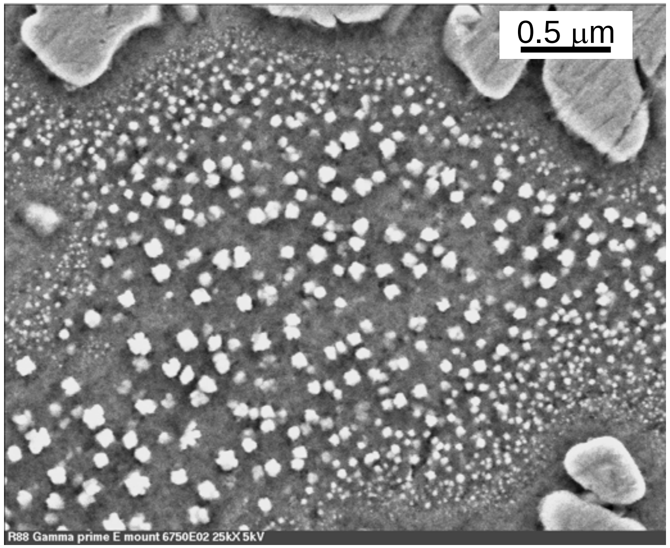
Interdiffusion Microstructures

Ni-Al-Cr





IN718 (S. Azadian et al.)



Disk alloy (courtesy of M.F. Henry)

Models/Software

- **1D Diffusion**
  - ✓ DICTRA
- **Mean-Field Precipitation**
  - ✓ PrecipiCalc
  - ✓ PanPrecipitation (PanSTAR)
  - ✓ TC-PRISMA
- **Phase Field – Most Feasible for Morphology Considerations**
  - ✓ MICRESS
  - ✓ PanROME

Modeling Challenges

- Multi-component, multi-phase, multi-variant and polycrystalline
- Very complex microstructural features:
  - ✓ high volume fraction of precipitates
  - ✓ non-spherical shape and strong spatial correlation
  - ✓ elastic interactions among precipitates
- Interdiffusion induces both microstructure and phase instabilities.
- Effect of concentration gradient on nucleation, growth and coarsening.
- Roles of defects and coherency/thermal stress on interdiffusion and phase transformation.
- Robustness and computational efficiency of models.

Phase Field Approach

$$\frac{\partial c(\vec{r},t)}{\partial t} = \nabla\left[M\nabla\frac{\delta F}{\delta c(\vec{r},t)}\right]$$

$$\frac{\partial \eta(\vec{r},t)}{\partial t} = -L\frac{\delta F}{\delta \eta(\vec{r},t)}$$

$$F(c,\phi) = \int_{\Omega}\left[f(c,\phi) + \frac{1}{2}\epsilon^2(\nabla\phi)^2 + \ldots\right]d\Omega$$

Phase Field Models

- Wheeler-Boettinger-McFadden(WBM)
  - ✓ *Phys. Review A, 45(10), 7424(1992)*
- MICRESS
  - ✓ Steinbach et al., *Physica D, 94, 135(1996)*
- Landau-Type Polynomial
  - ✓ L.Q.Chen and Y. Wang, *JOM, 48, 13-18(1996)*
- Kim-Kim-Suzuki(KKS)
  - ✓ *Phys. Review E, 60(6), 7186(1999)*

Kim-Kim-Suzuki(KKS) Model

Local Free Energy Density

$$f(c,\phi) = h(\phi) f^S(c_S) + [1 - h(\phi)]\, f^L(c_L) + g(\phi)$$

$$h(\phi) = \phi^3 \left(6\phi^2 - 15\phi + 10\right)$$

$$g(\phi) = \omega \phi^2 (1 - \phi)^2$$

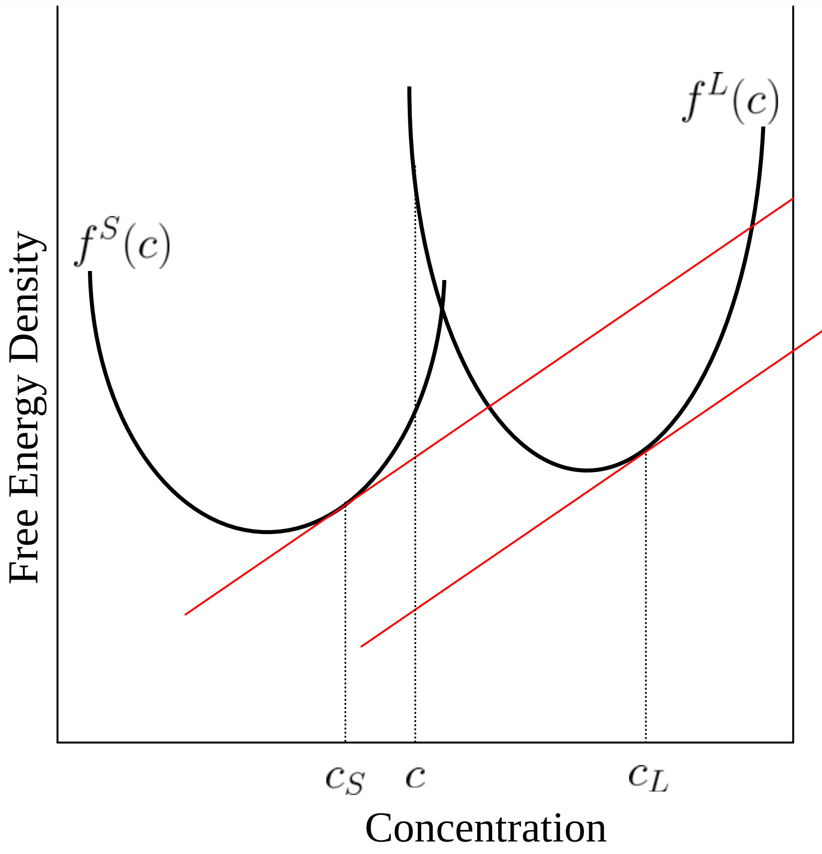
Kim-Kim-Suzuki(KKS) Model

Mass Conservation

$$c = h(\phi)c_S + [1 - h(\phi)]\, c_L$$

Equal Diffusion Potential

$$f^S_{c_S}\left[c_S(x,t)\right] = f^L_{c_L}\left[c_L(x,t)\right]$$



Advantage of KKS Model

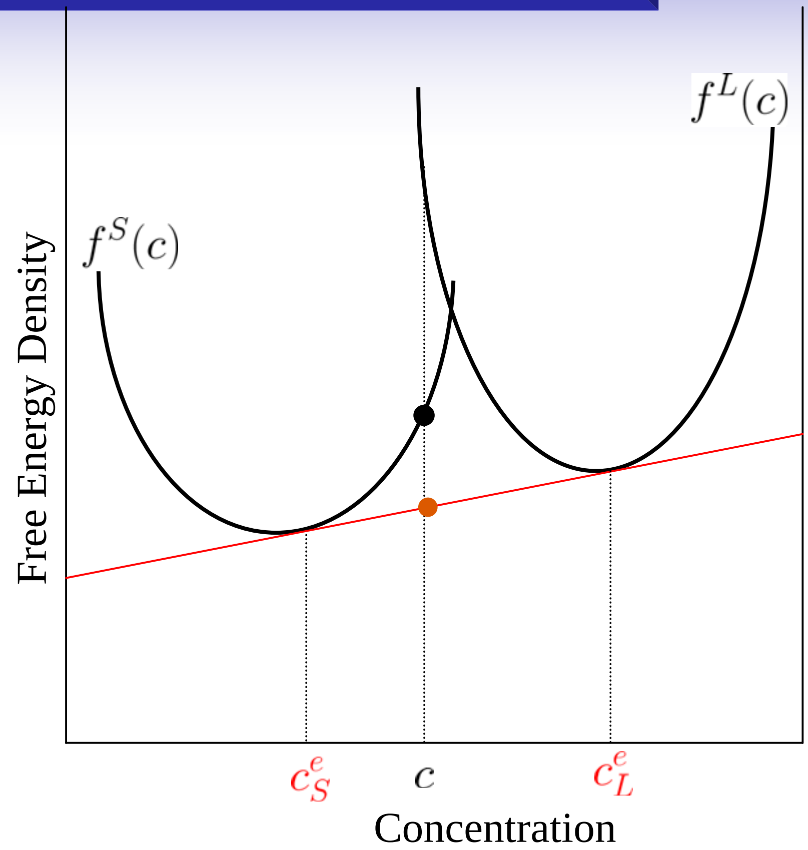
Adjustable Interfacial Energy

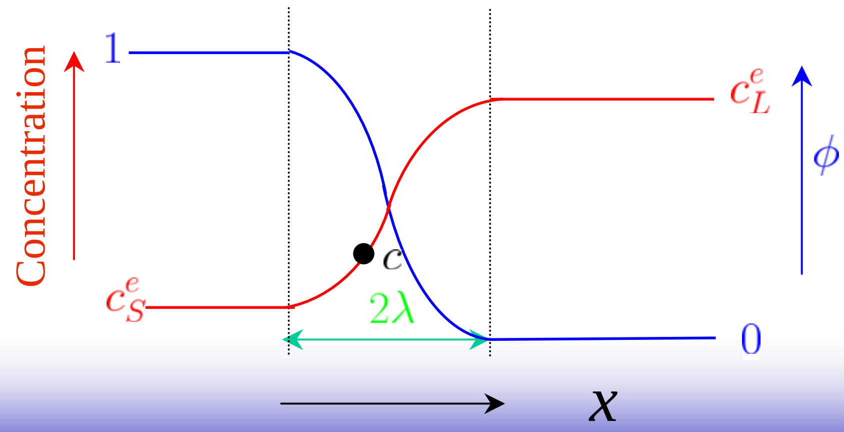
Practical Length Scale

$$\sigma = \frac{\epsilon\sqrt{\omega}}{3\sqrt{2}}$$

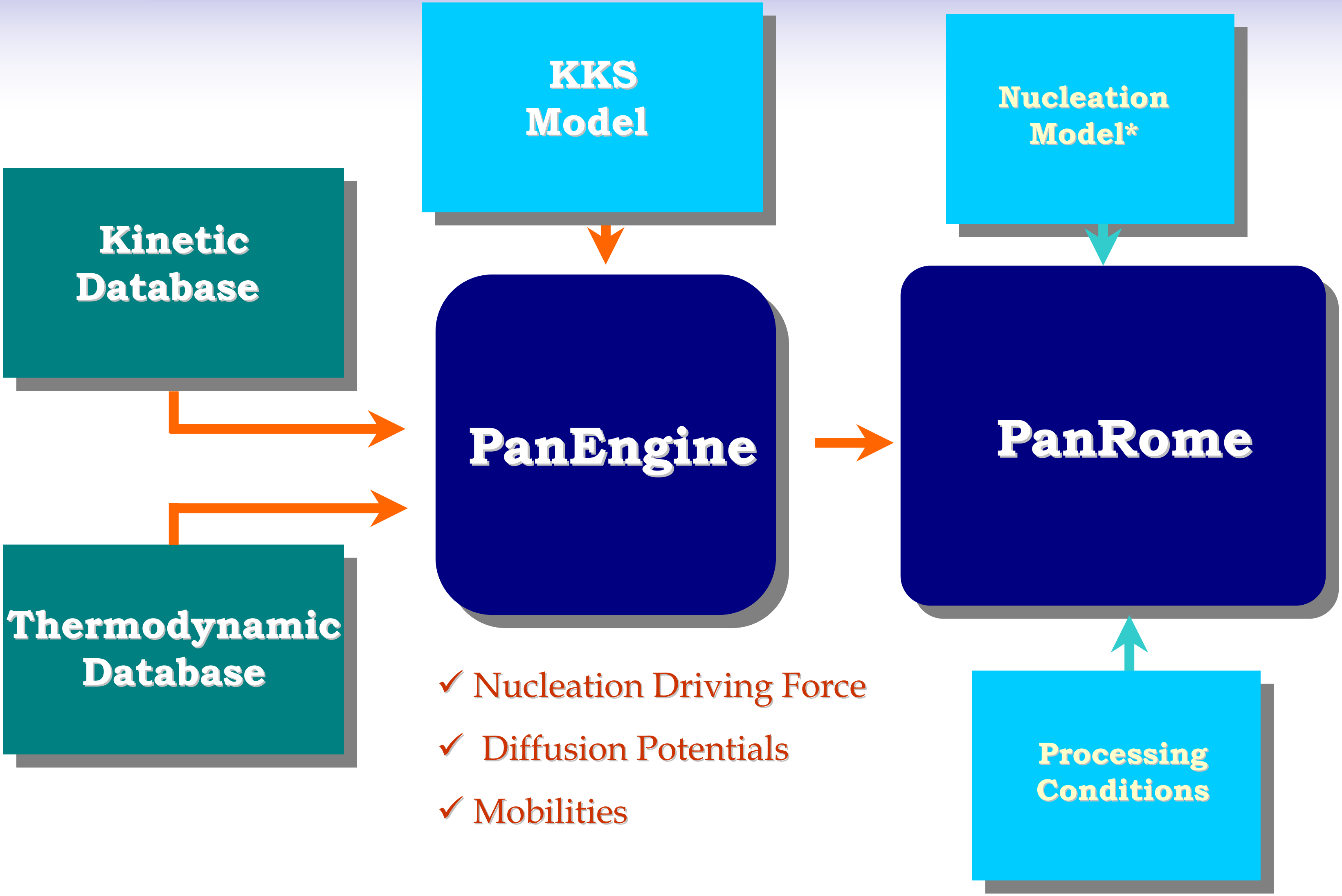
$$2\lambda = \alpha\sqrt{2}\frac{\epsilon}{\sqrt{\omega}}$$

$$\alpha \approx 2.2 - 2.94$$





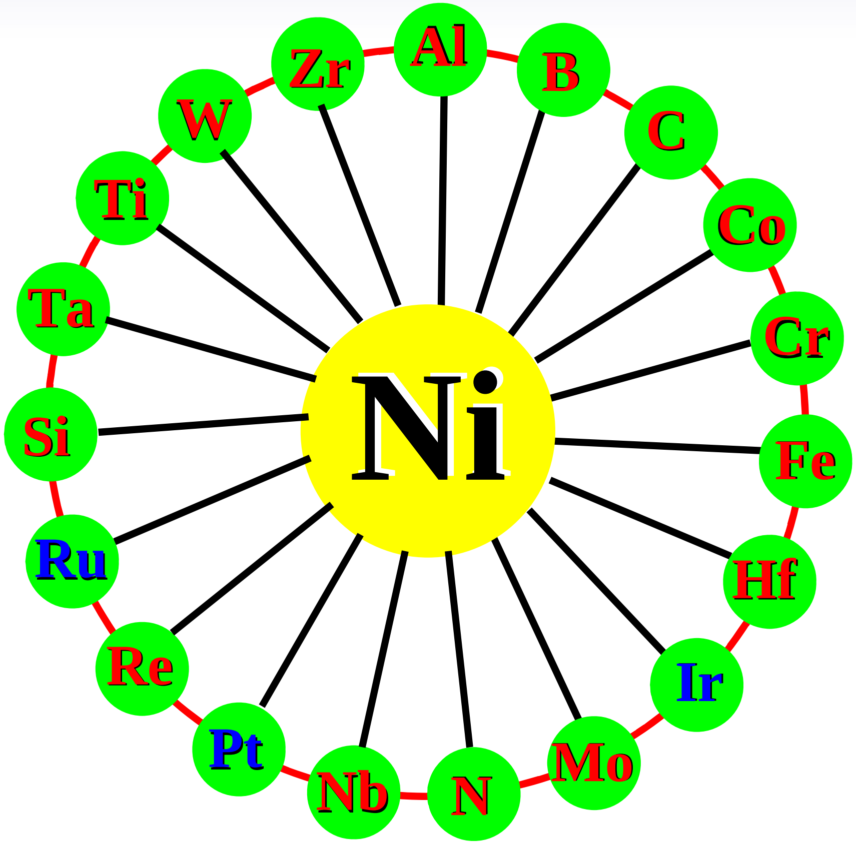
Software Architecture



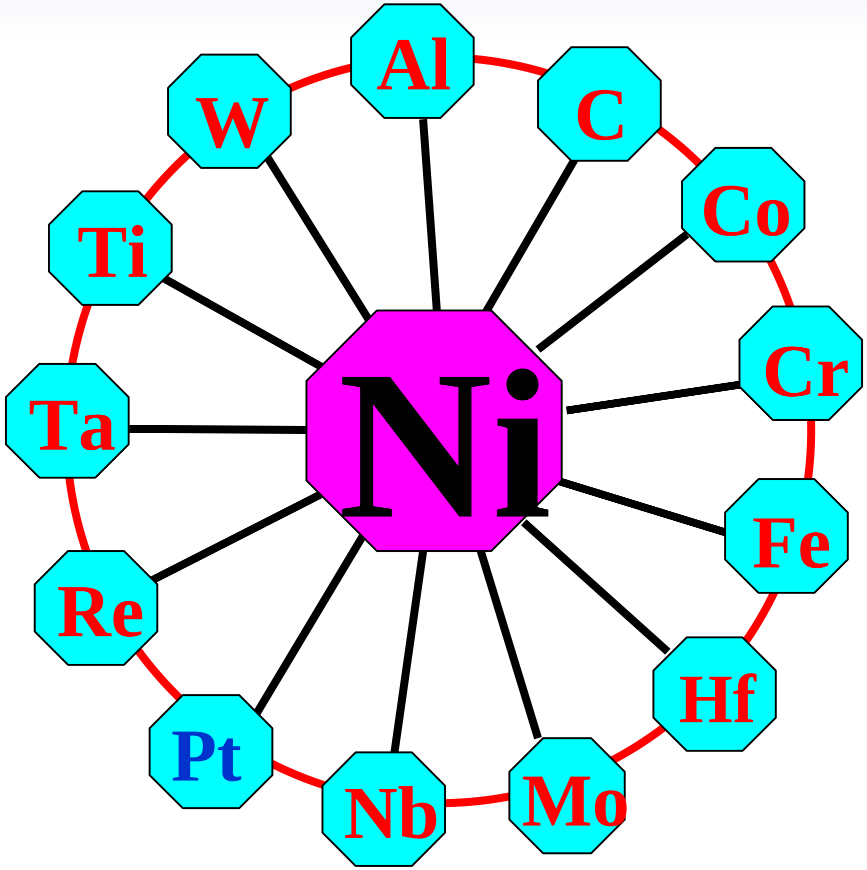
*C.Shen, Ph.D. Thesis, The Ohio State University, 2004;

Y.H. Wen et al., *Acta Mater.*, 51, 1123(2003)

Ni Databases



Thermodynamic



Kinetic*

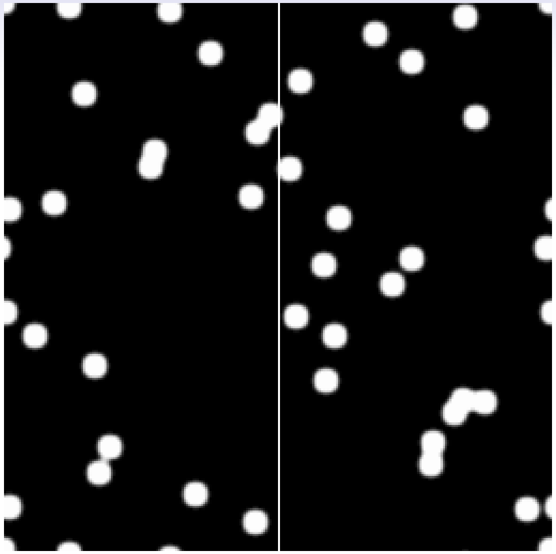
* Partly from C. E. Campbell, W. J. Boettinger, U. R. Kattner, *Acta Mater*. 50, 2002, 775-792.

Coarsening

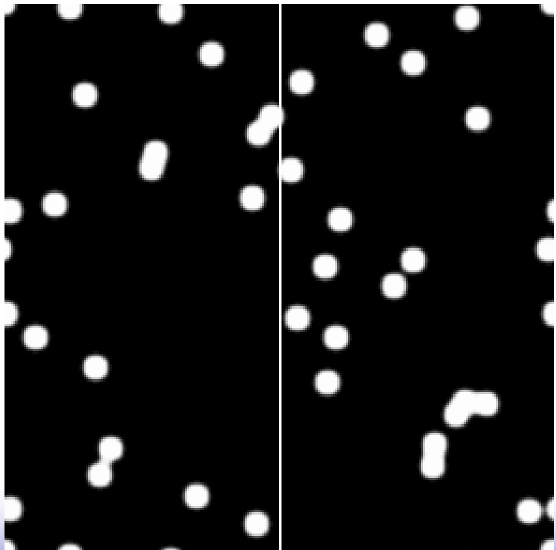
Ni-Al-Cr-Pt

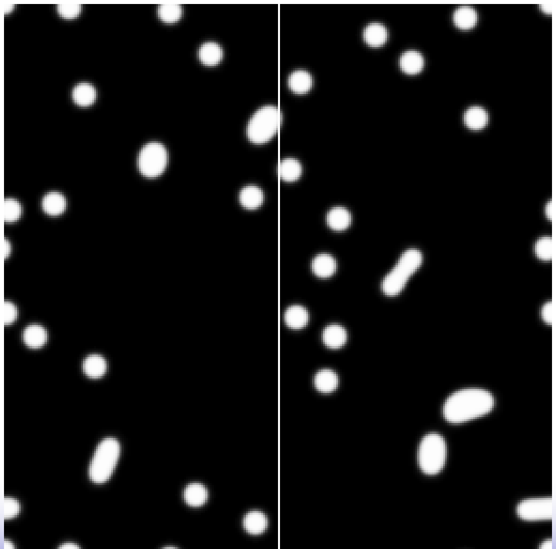
$\gamma+\gamma'$

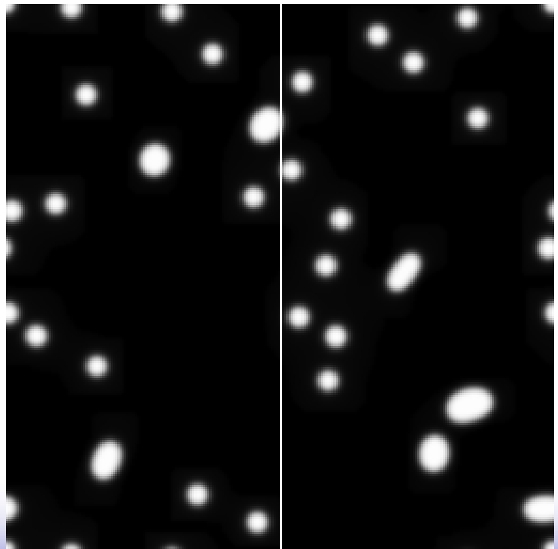
1200°C 500hrs



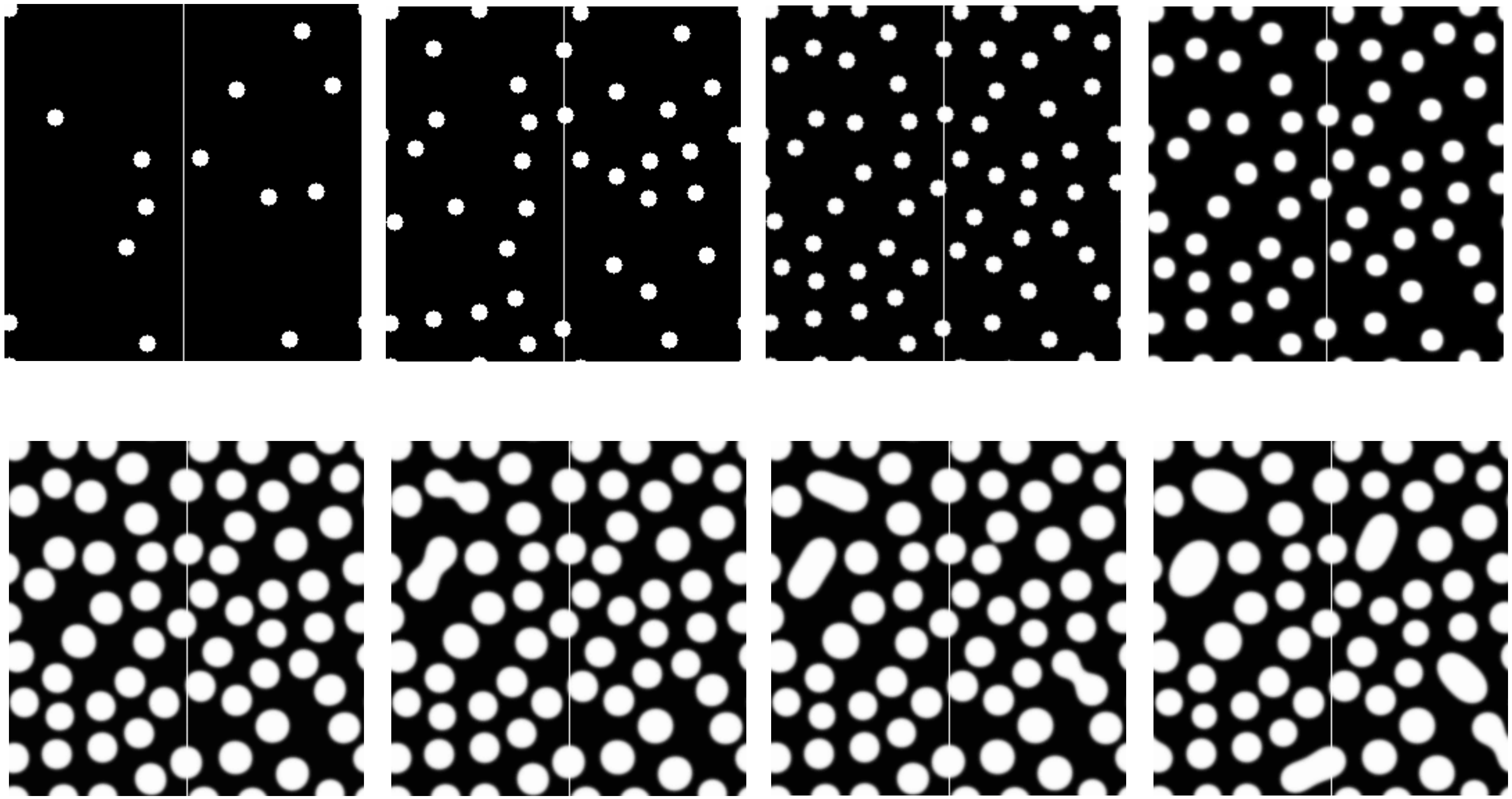
$$\sigma_1 < \sigma_2 < \sigma_3$$





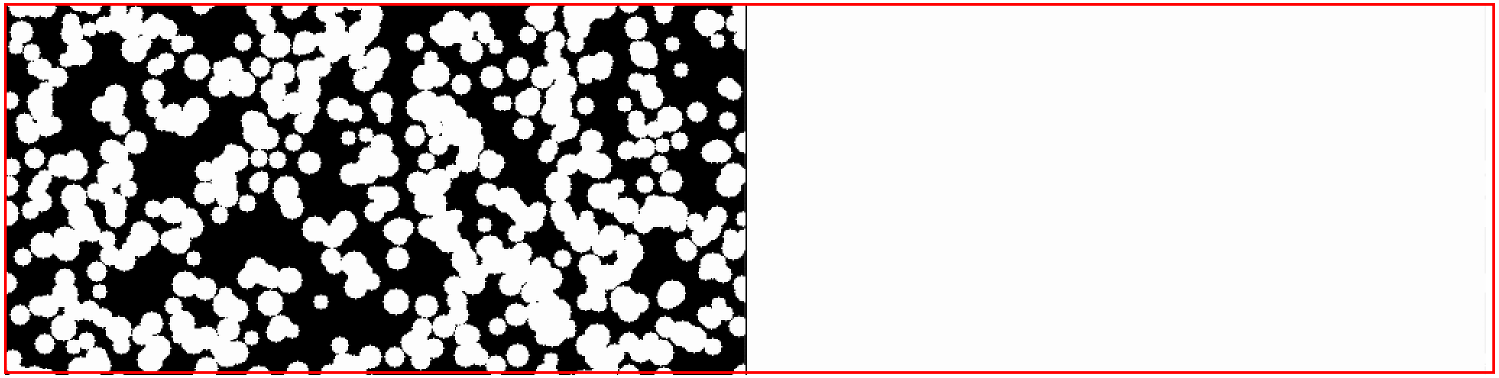


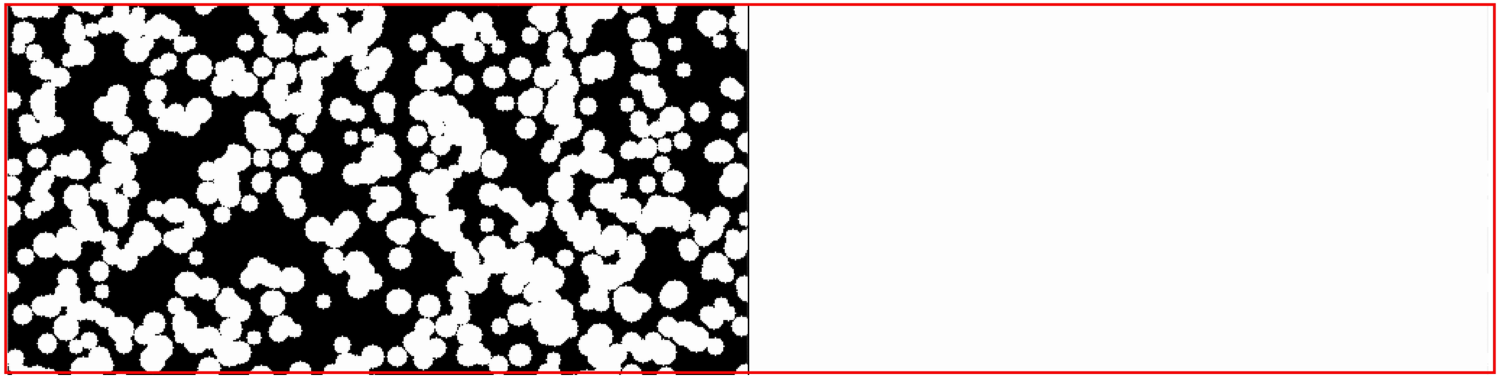
Nucleation



β+γ/γ Diffusion Couple

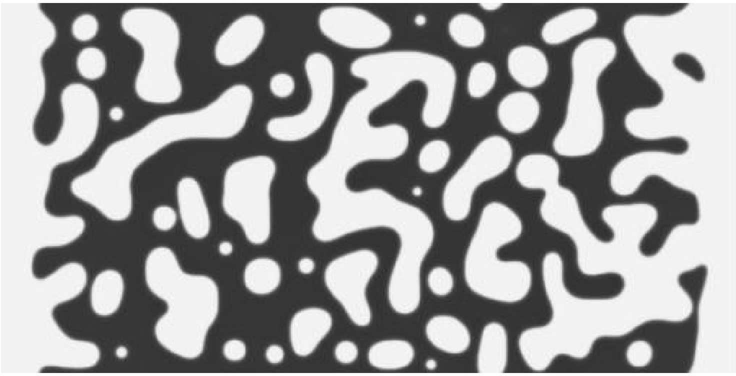
Ni-Al-Cr



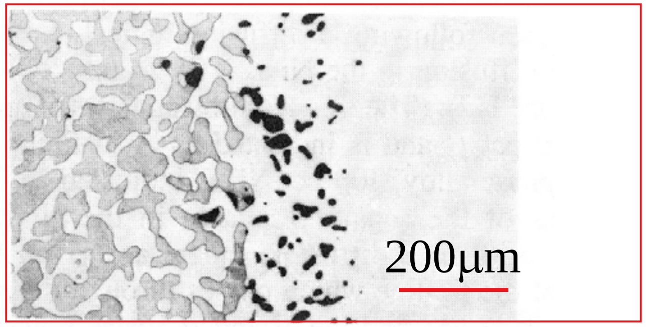


β+γ/γ Diffusion Couple

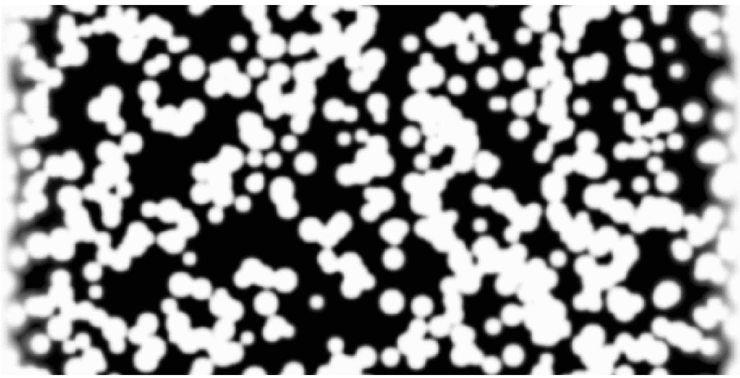
Landau-Type Polynomial

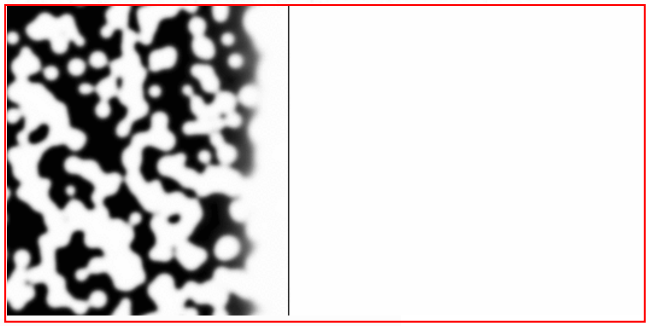


*Exp. Observation**
100 hrs at 1200°C



Kim-Kim-Suzuki Model





*J.A.Nesbitt and R.W.Heckel, *Metall. Trans. A,* 18A(11)2087(1987)

Software

- Coded in C++ & provided as a Windows dll
- Script file for user inputs
- ImageMagick for microstructure images
- Pandat GUI under development

Computational Efficiency

- A special algorithm/data structure is designed to improve the efficiency
- Benchmark:
  - ✓ Computer : Intel Core2 Duo CPU 3.0GHz, 3G Memory
  - ✓ System: Ni-Al-Cr, $\beta+\gamma/\gamma$ diffusion couple, 1024×256 grid points, 300hrs annealing time at 1200^{o}C

Simulation Time : 24 hrs

Summary

- A phase field program for interdiffusion microstructures
- Introduction of Kim-Kim-Suzuki model to relax the restriction of the length scale
- Examples demonstrating feasibilities
- Computational efficiency

Future Work

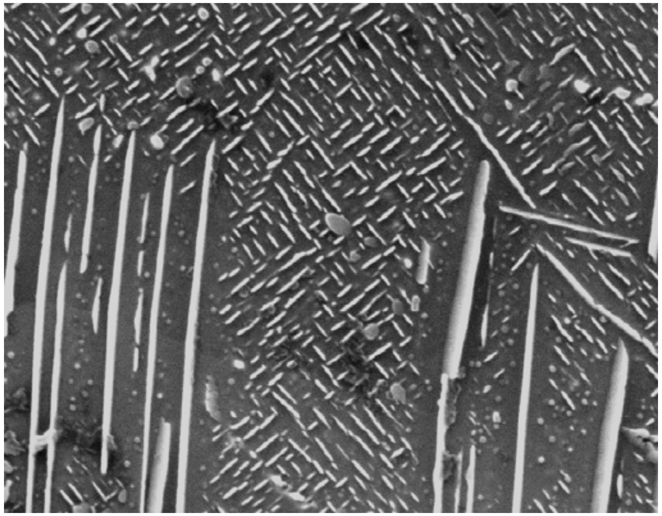
More Validations

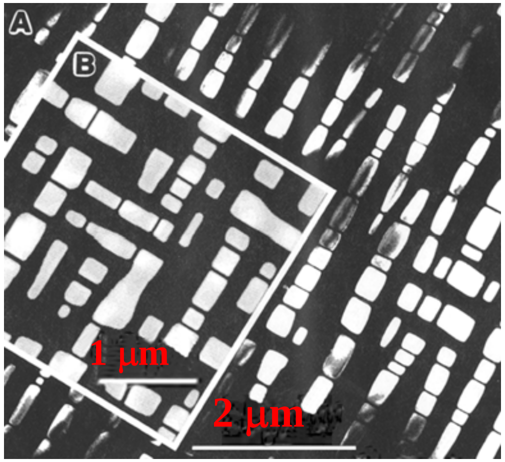
- Non-isothermal conditions
- Multiphase systems
- More than 4 components
- Different alloy systems

Future Work

More Functionalities

- Interfacial energy anisotropy
- Elastic strain energy effect

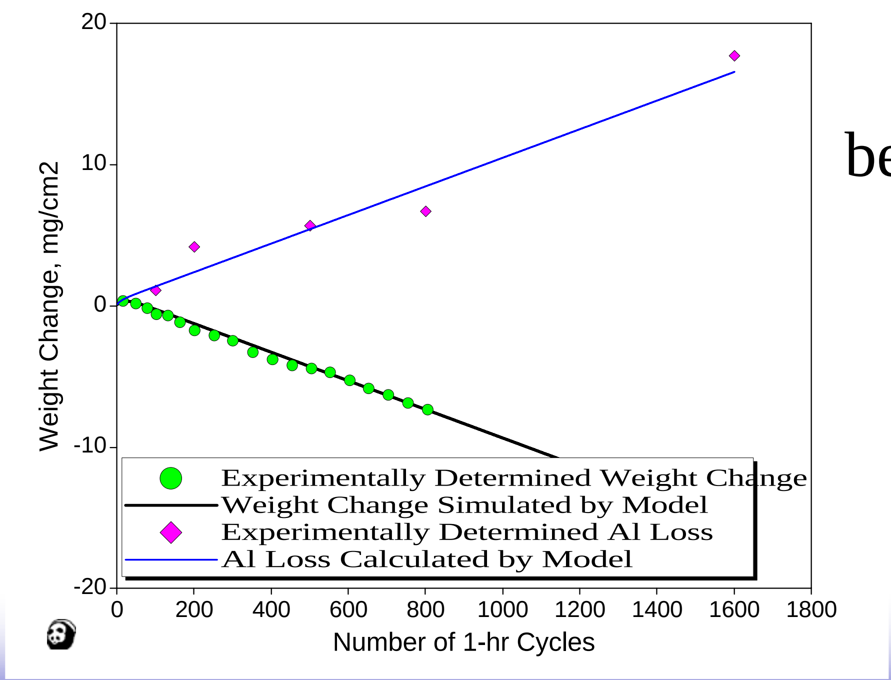




Future Work

More Boundary Conditions

- ➢ CVD Processing
- ➢ Oxidation (Integrated with COSP)



Oxidation behavior of a $\gamma+\beta$ alloy