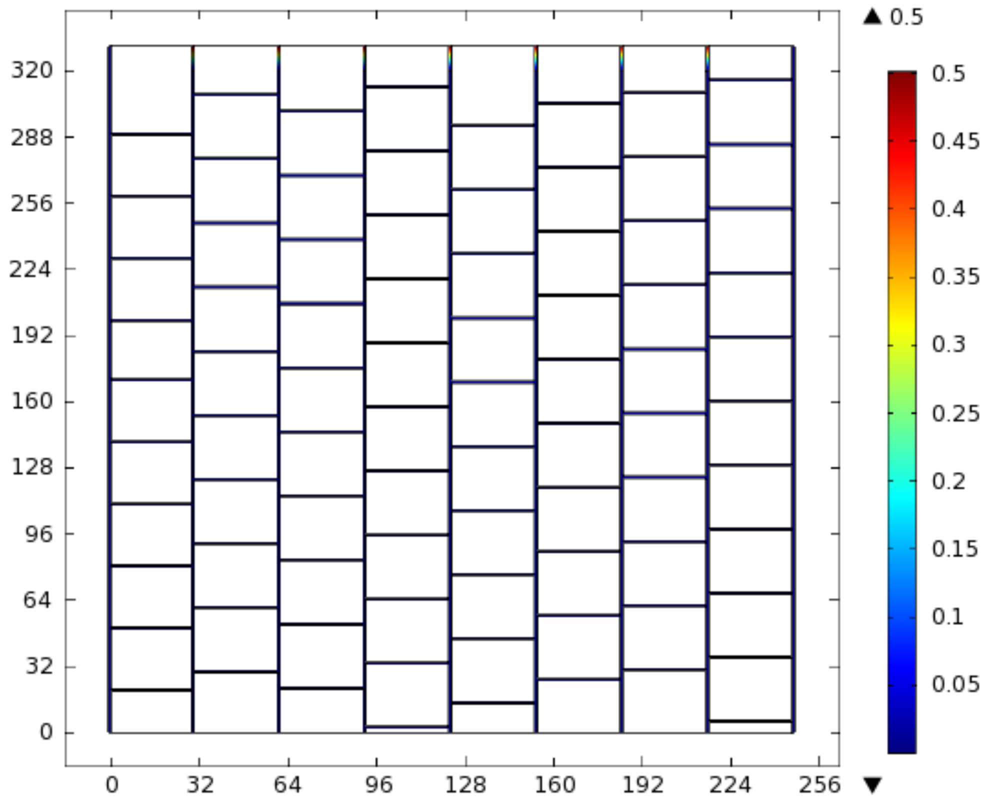
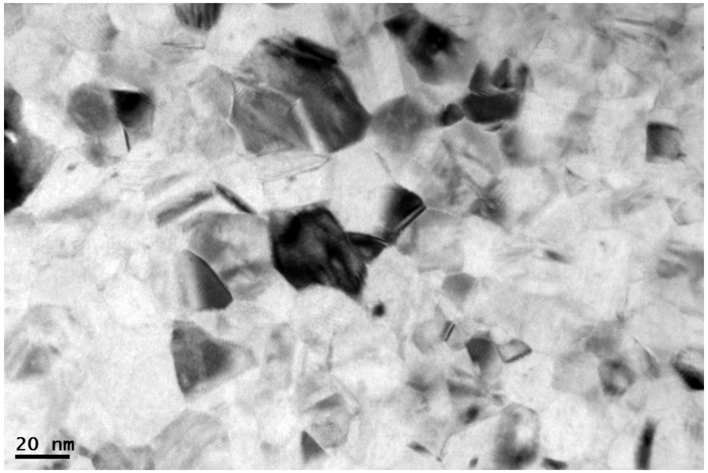
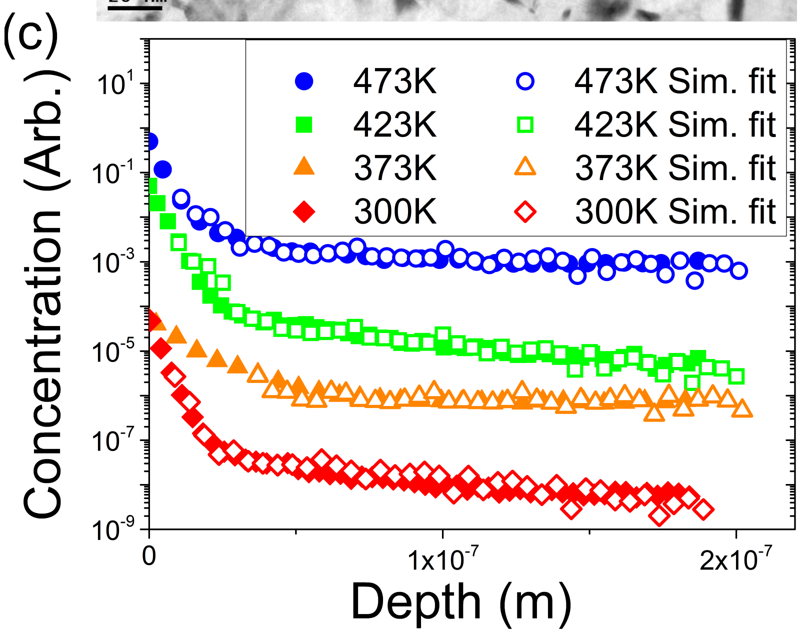
Finite Element Simulation

Grain boundary diffusion in thin film model:

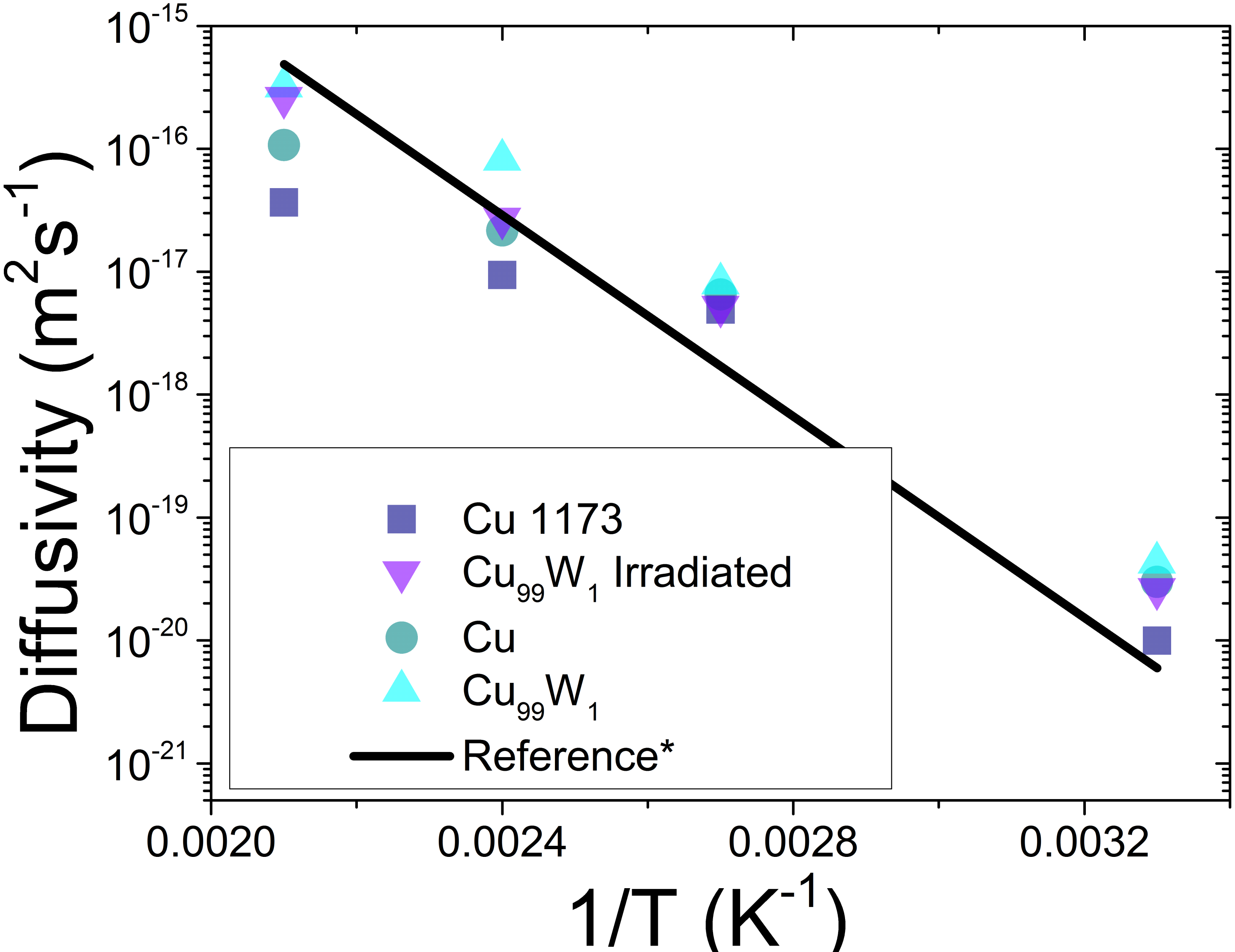
Near surface (10~20nm) D_{sb} different from $D_b$in film







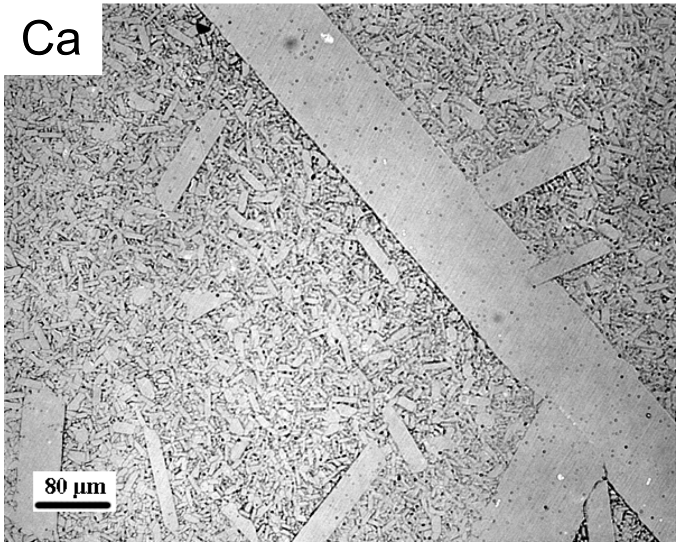
Results of Au G.B. Diffusion in Cu

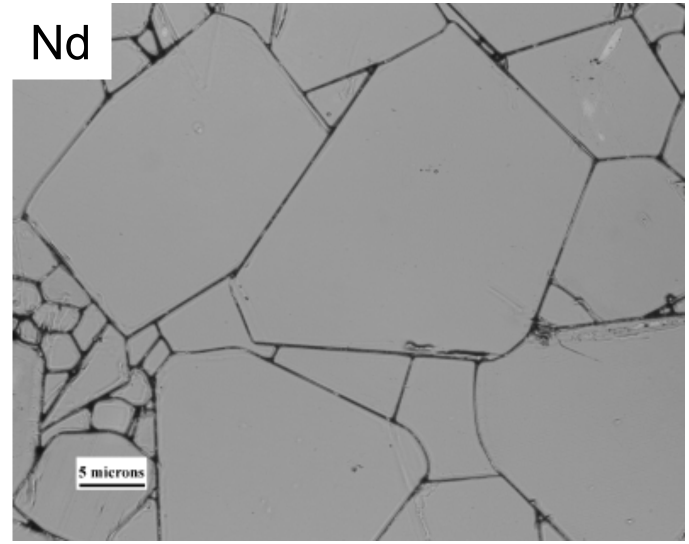


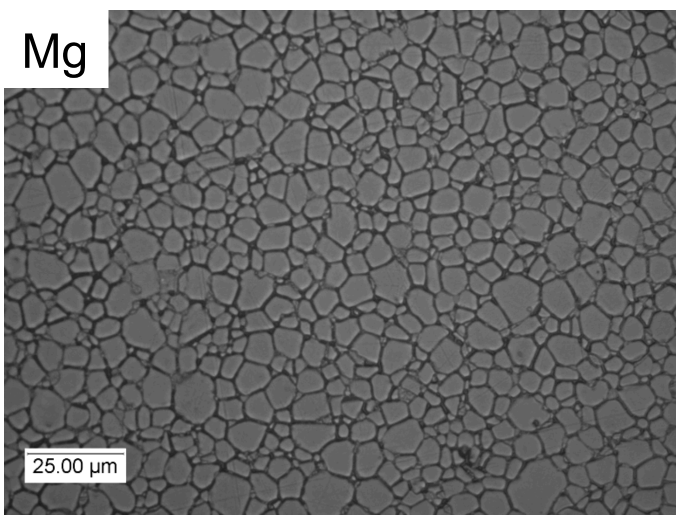
Au diffusivity in the Cu – Limited 'nano-effect'

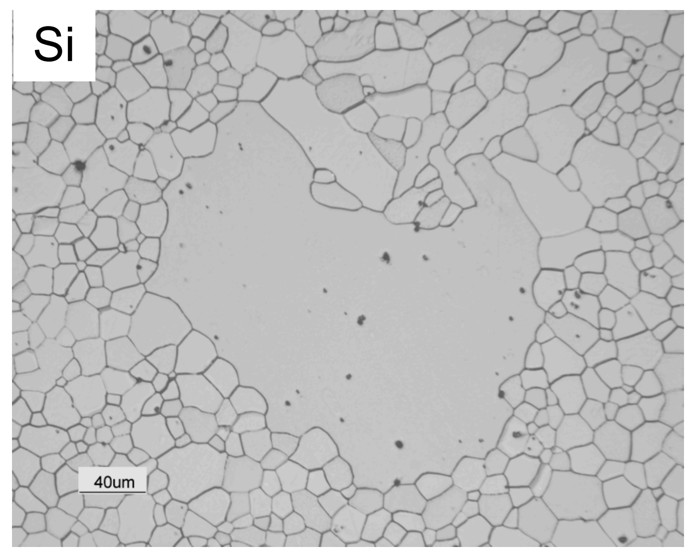
*Ref. Surholt, Mishin, Herzig, *Phys. Rev. B* (1994).

Aluminum Oxide

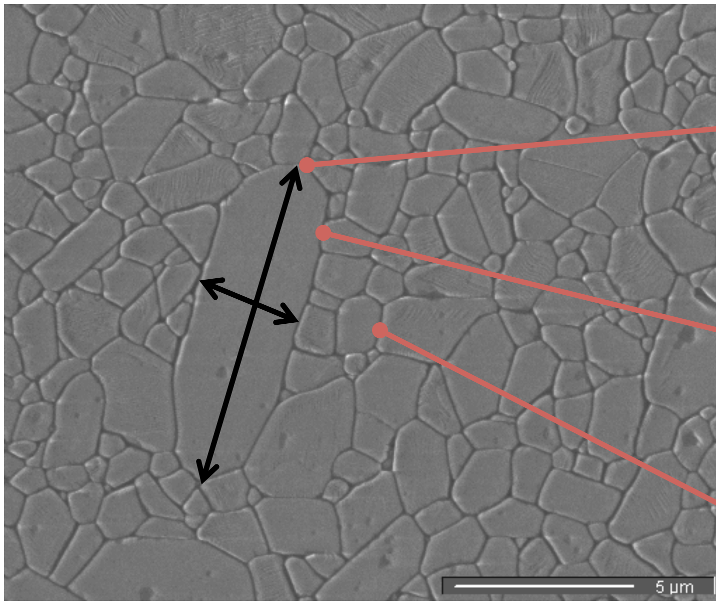


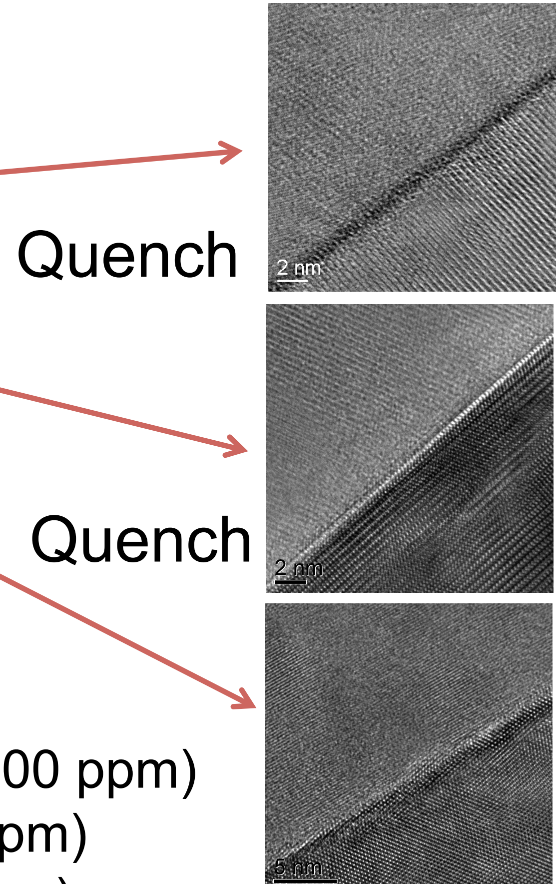






Experimental Approach





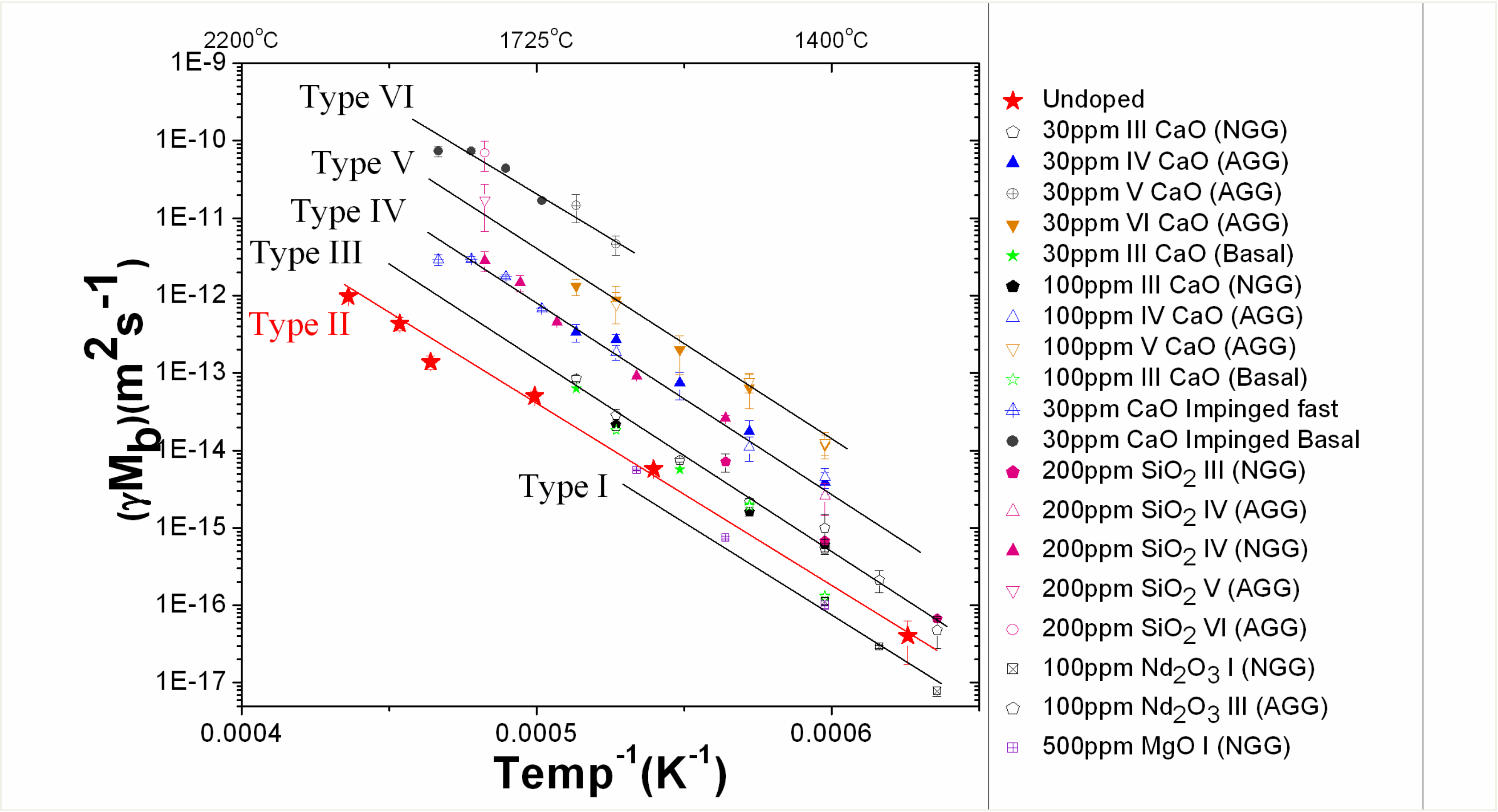
TEM

Compositions Investigated

- Calcia-doped Alumina (30, 100, 500 ppm)
- Silica-doped Alumina (200, 500 ppm)
- Magnesia-doped Alumina (500 ppm)
- Neodymia-doped Alumina (100 ppm)

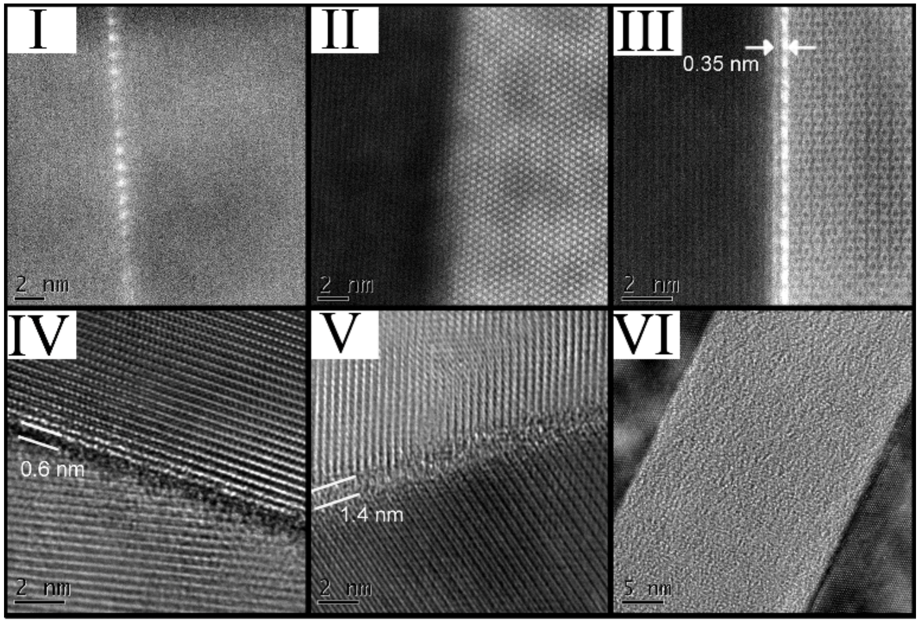
Wide Temperature Range: 1300-2020^{o}C

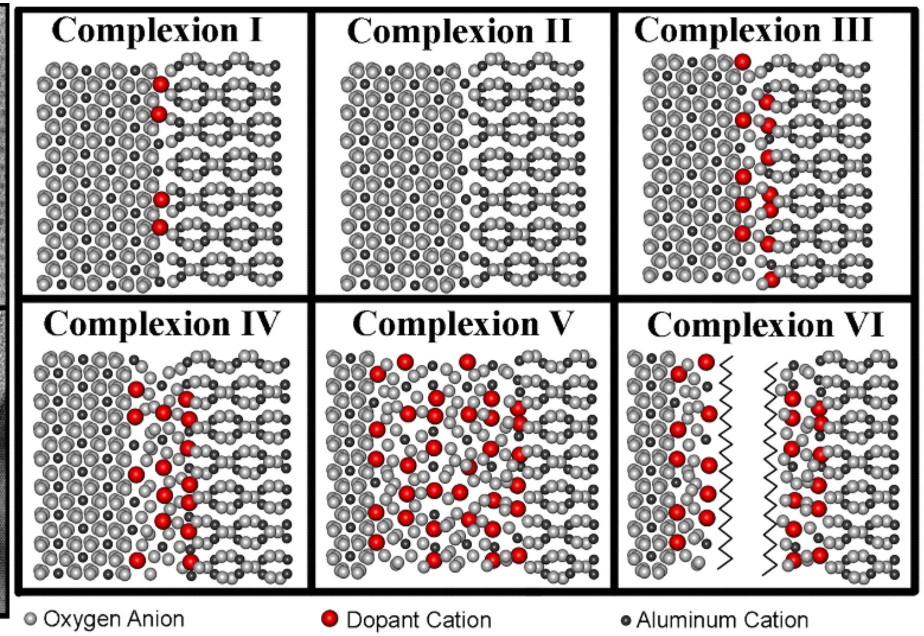
Grain Growth Kinetic Types



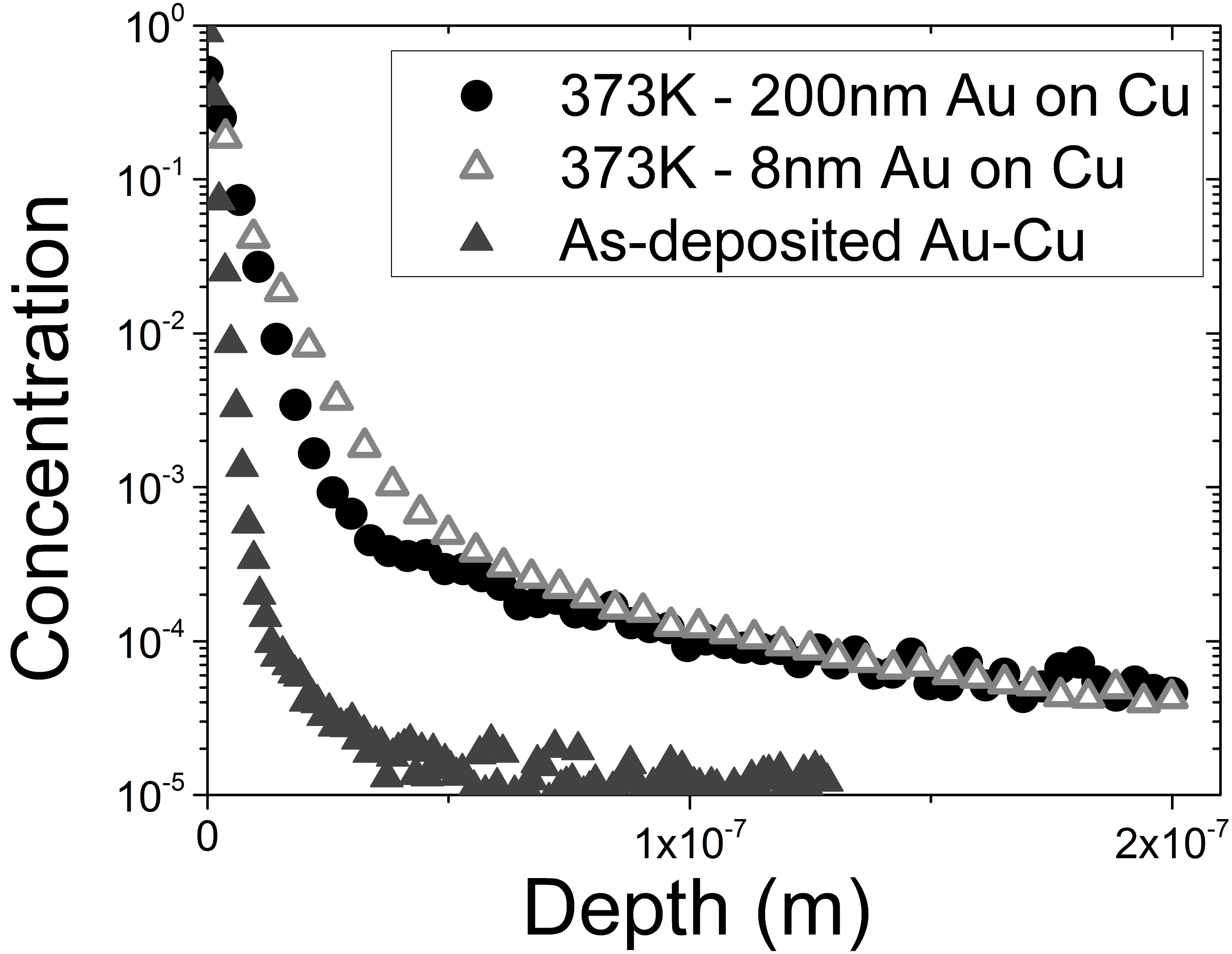
S.J. Dillon, M. Tang, W.C. Carter, M.P. Harmer, "Complexion: A new concept for kinetic engineering in materials science," *Acta Mater.* 55[18] 6208-6218 (2007)

Nanoscale Interface Structure



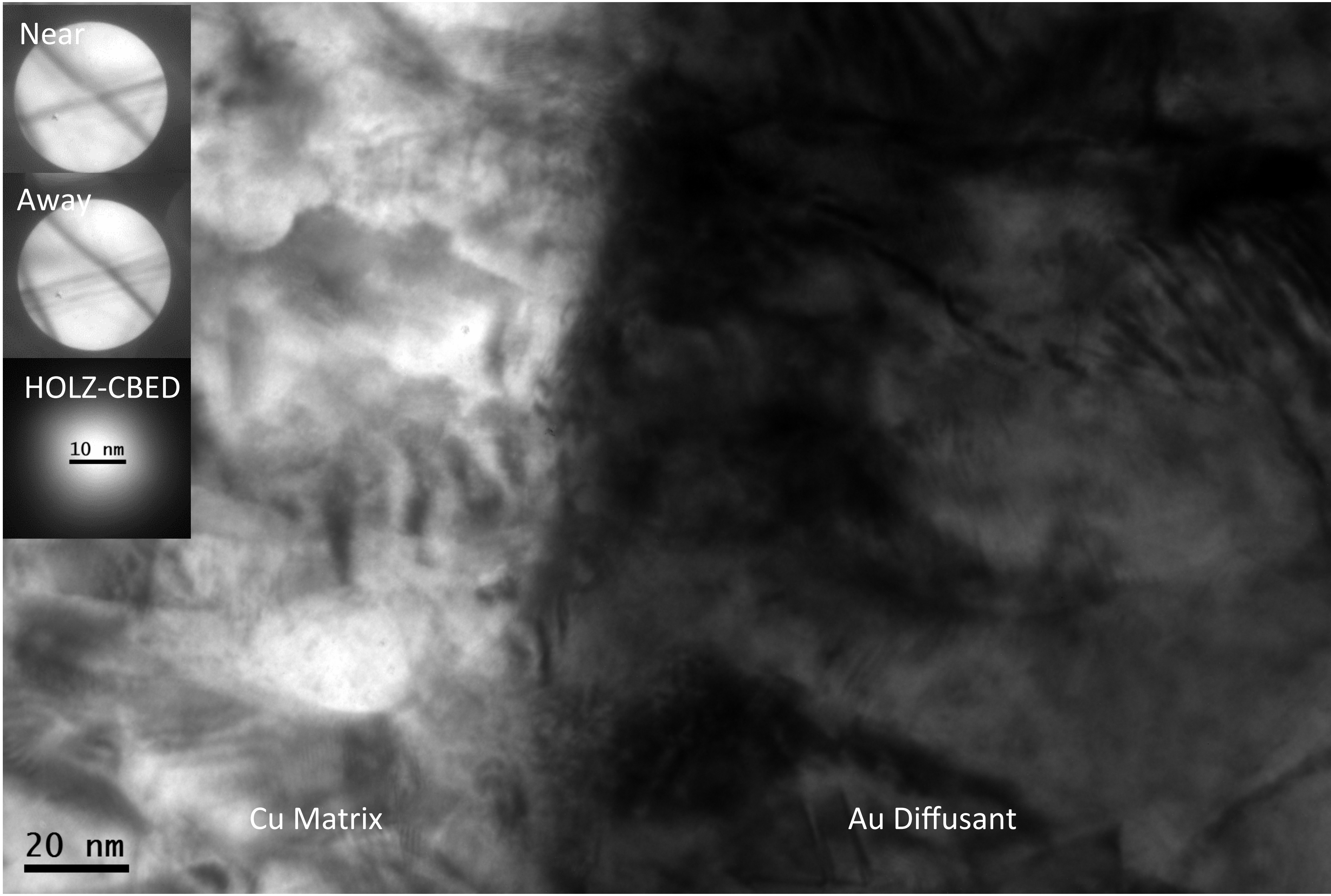


Variation in structure on nano-scale can produce orders of magnitude changes in properties



Concentration
Depth (m)
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
0
1x10^-7
2x10^-7
373K - 200nm Au on Cu
373K - 8nm Au on Cu
As-deposited Au-Cu

Stress at Interface



Model for Equiaxed Nanograins

Type B

Constant Source

$$sD_{gb}\delta = 1.308\sqrt{\frac{D}{t}}(-\partial\bar{c}/\partial z^{6/5})^{-5/3}$$

Modified 'Type B'-like model

Constant Source

$$D_{gb}\delta = 1.308\sqrt{\frac{D^{eff}J}{t}}\left(-\partial\bar{c}/\partial z^{6/5}\right)^{-5/3}$$

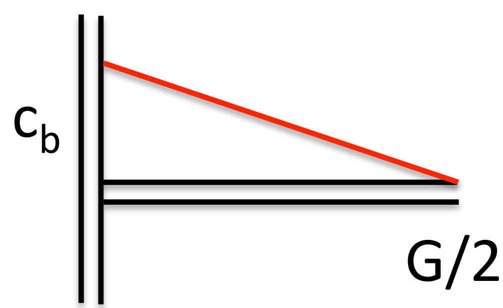
Correction Factor, J

Motivation – Basis of Type B

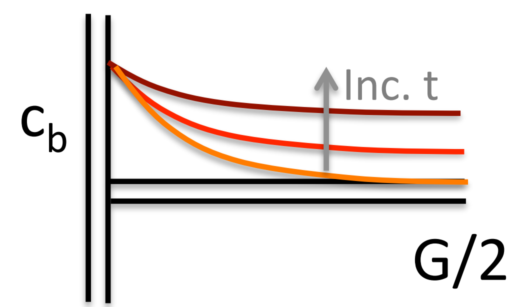
$$\frac{\partial c_b}{\partial t} = D_b\frac{\partial^2 c_b}{\partial x^2} - J\frac{2D}{\delta}\frac{\partial c_g}{\partial r}\bigg|_{r=r_b}$$

$$J = \frac{\int D(\partial c/\partial x)\,dt}{\int D(\partial^2 c/\partial x^2)\,dt}$$

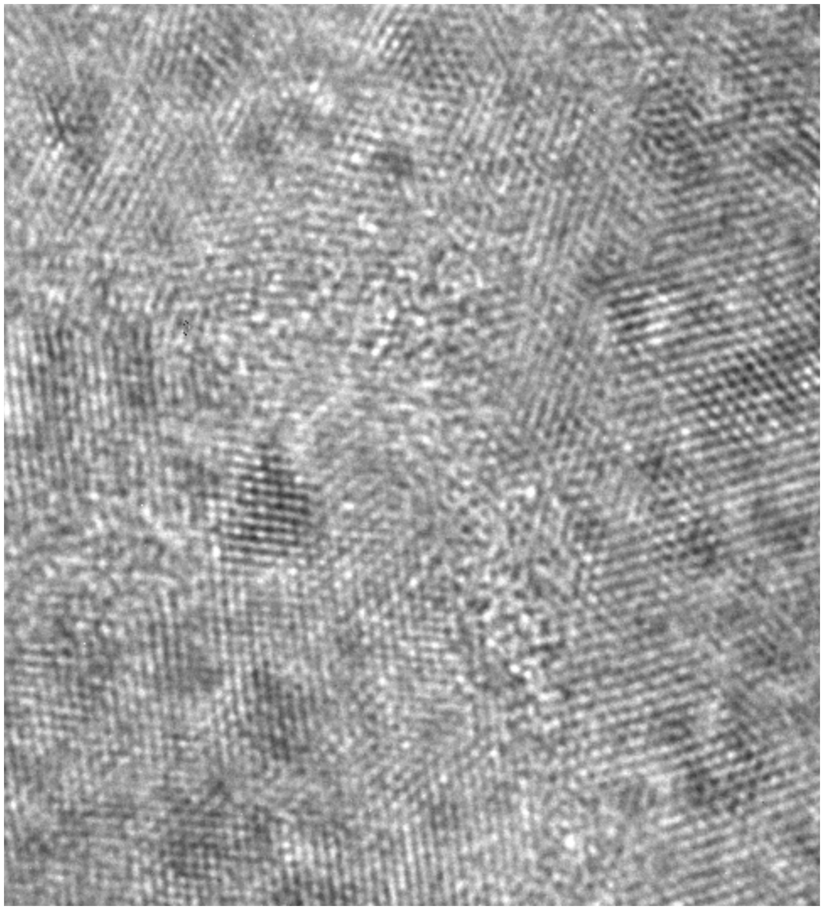
$$\partial c/\partial t = D(\partial c/\partial x)$$

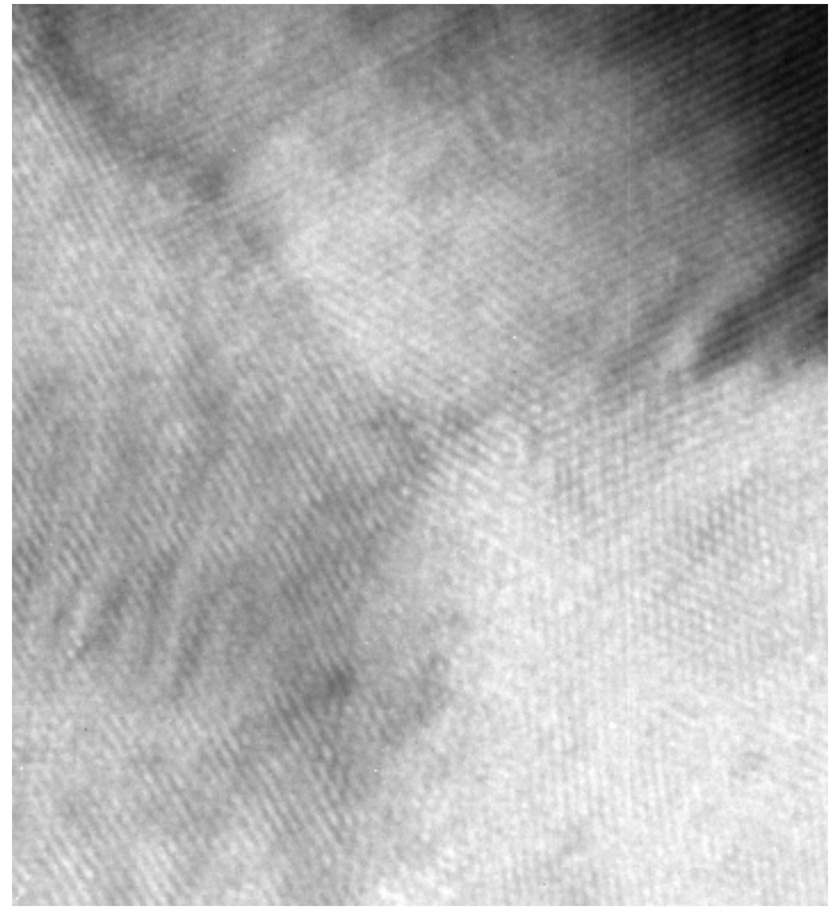


$$\partial c/\partial t = D(\partial^2 c/\partial x^2)$$



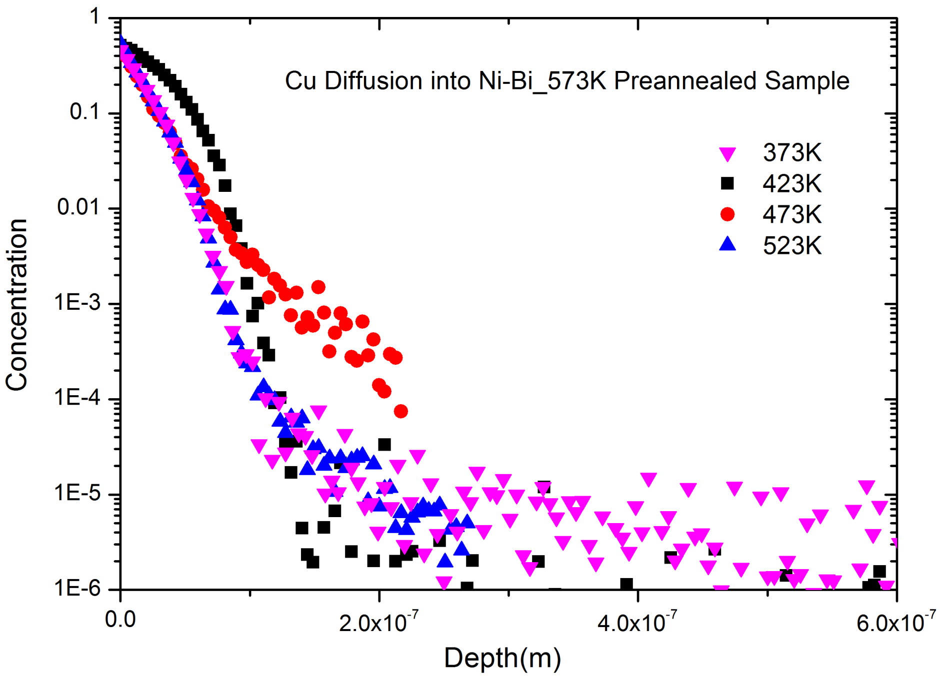
Disorder-Order Transition Irradiated Cu-W



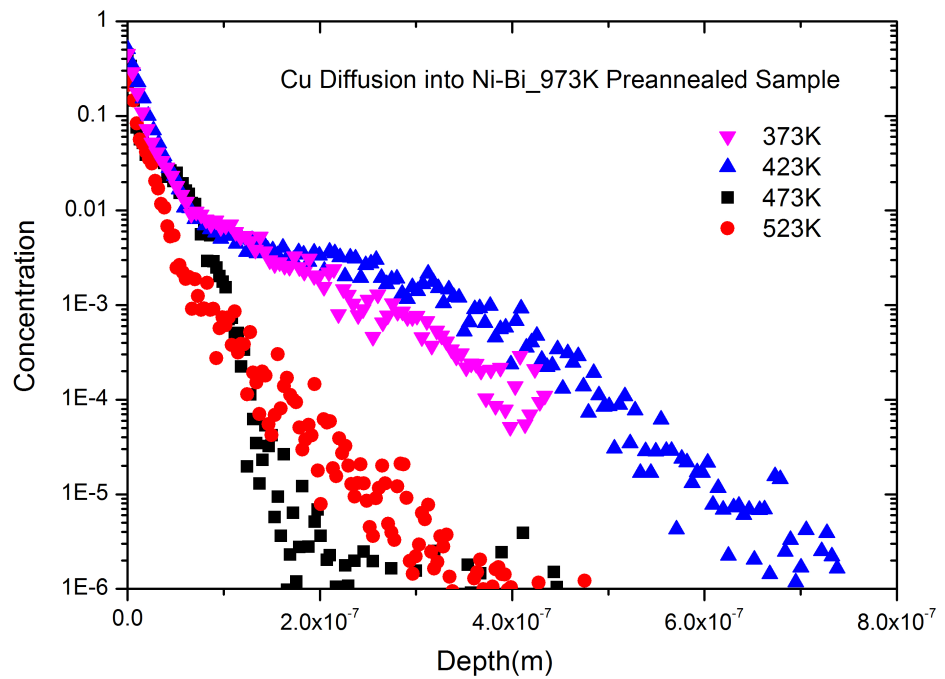


Cu diffusion into Bi-doped Ni Matrix

Low T pre-anneal 300^{o}C



High T pre-anneal 700^{o}C

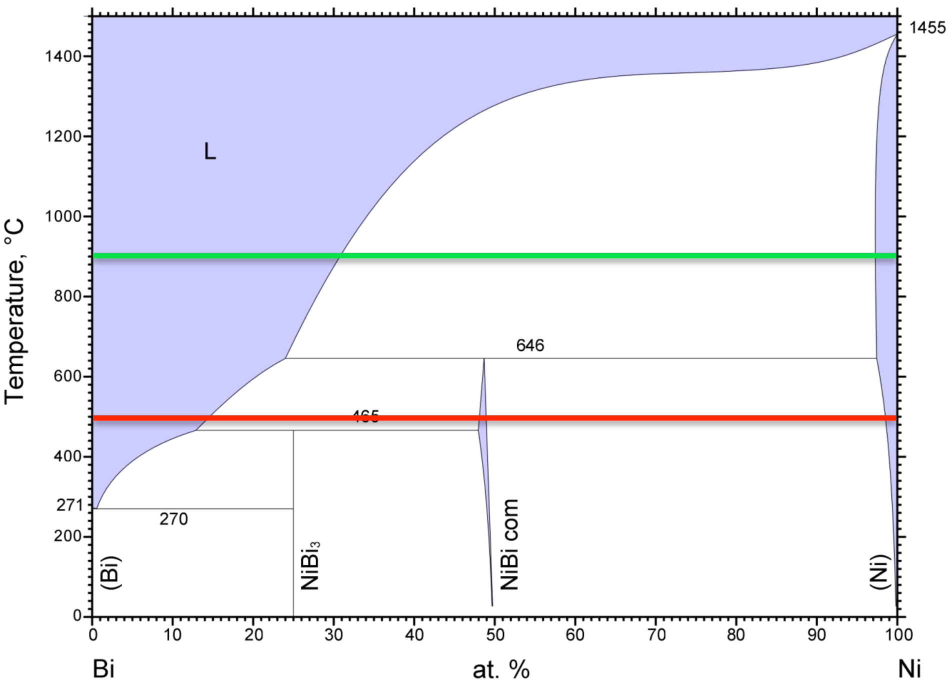


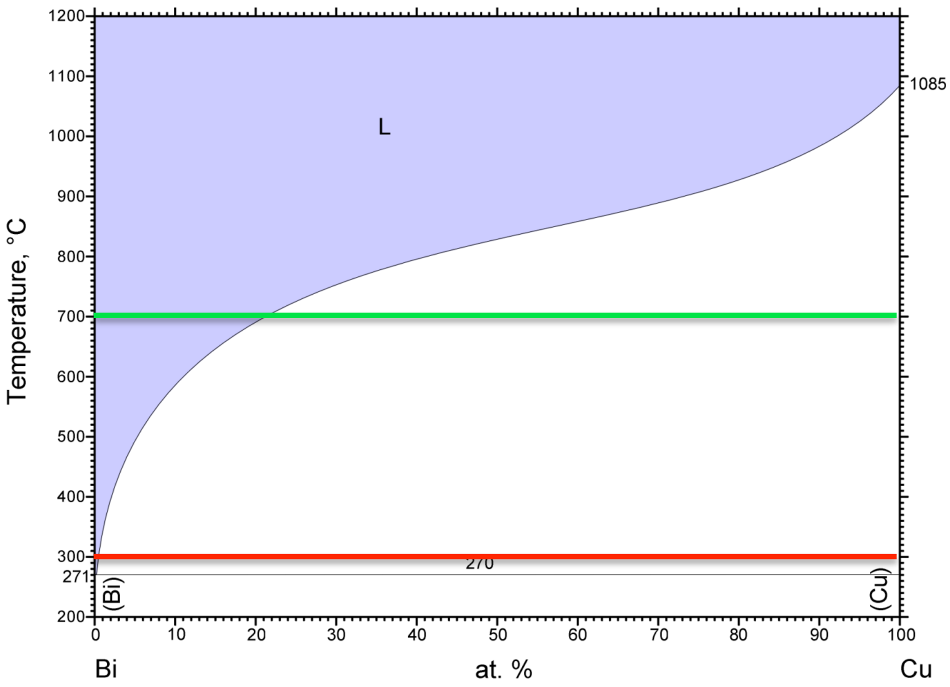
Comparison of 2 Model Systems

Miedema Model:

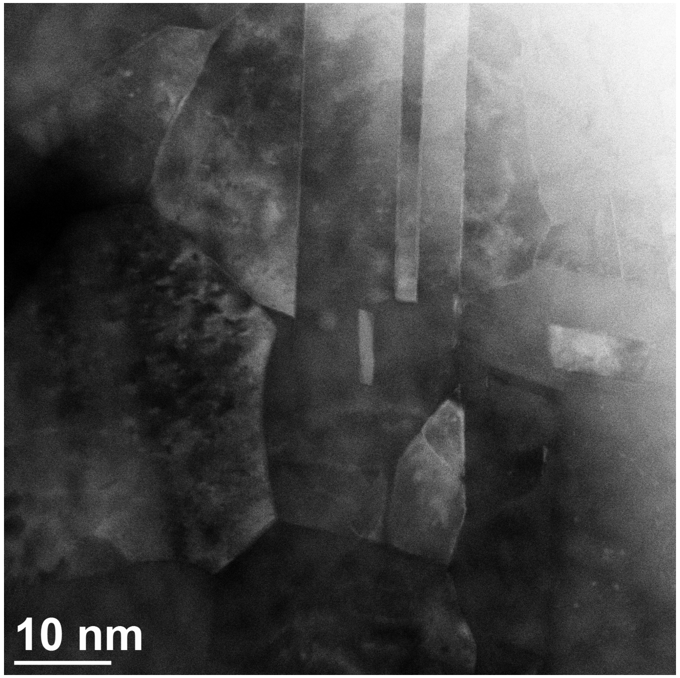
$\Delta H_{mix}^{(50\%Ni\text{-}50\%Bi)}$ = -3.7 kJ/mol

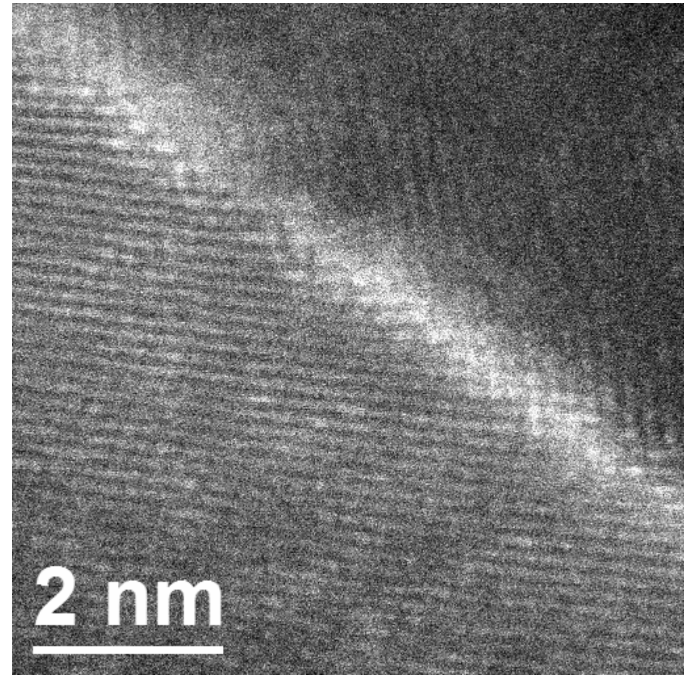
$\Delta H_{mix}^{(50\%Cu\text{-}50\%Bi)}$ = +3.56 kJ/mol

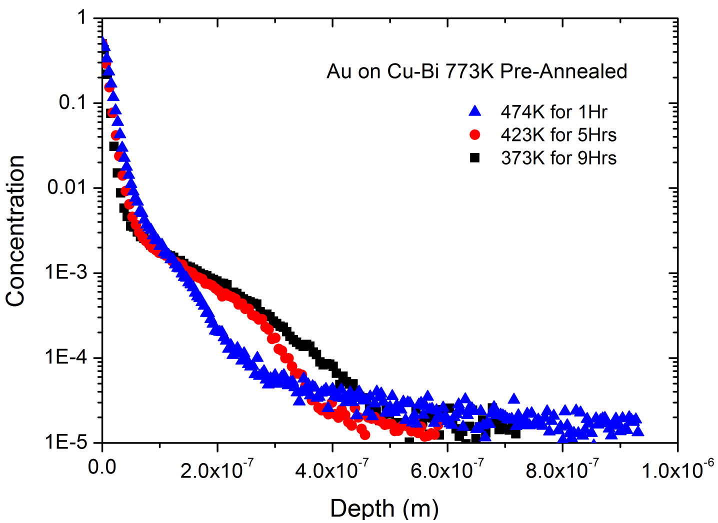




500 ºC Pre-annealed with Bi

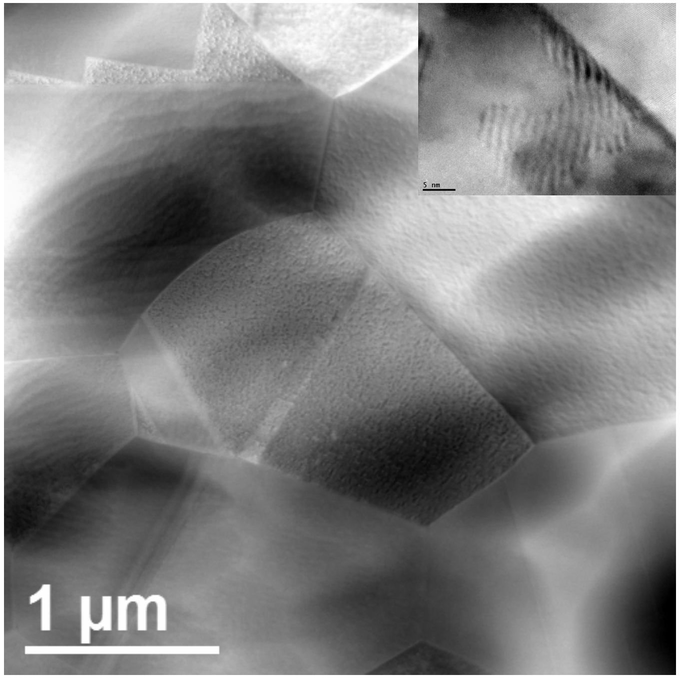


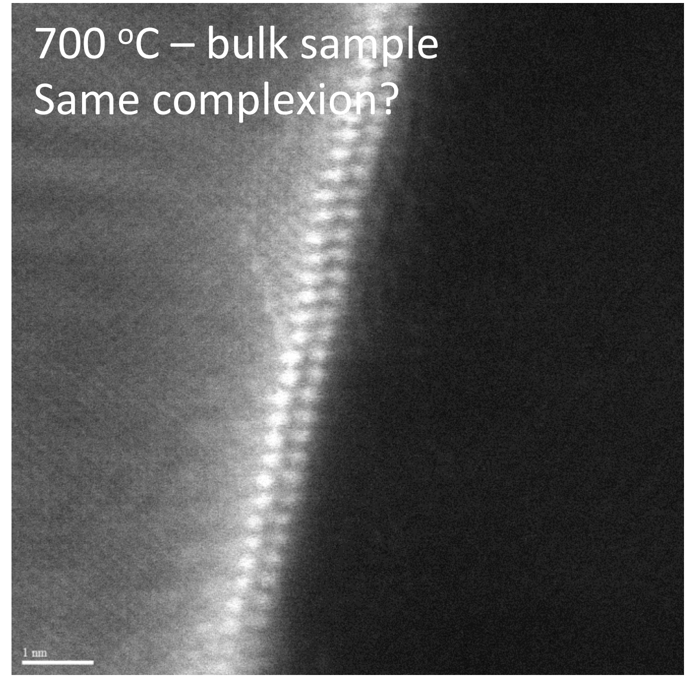


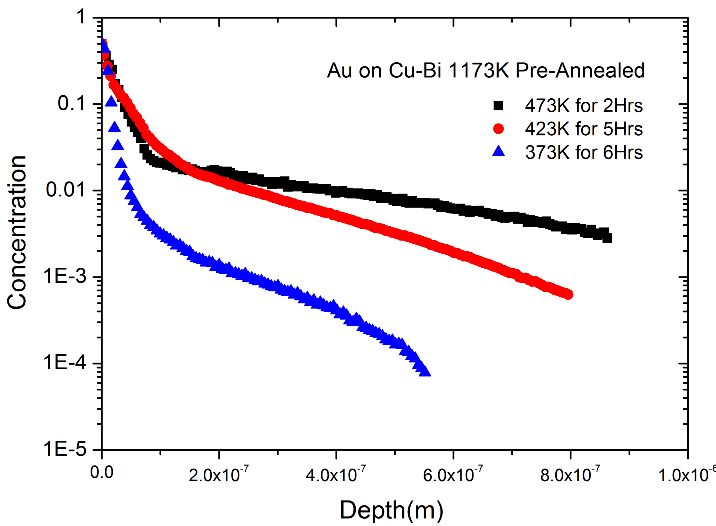


$$\bar{c}(z) \approx \bar{c}_{gb}(z) \propto \mathrm{erfc}\left(\frac{z}{2\sqrt{D_{gb}t}}\right)$$

900 °C Pre-annealed with Bi

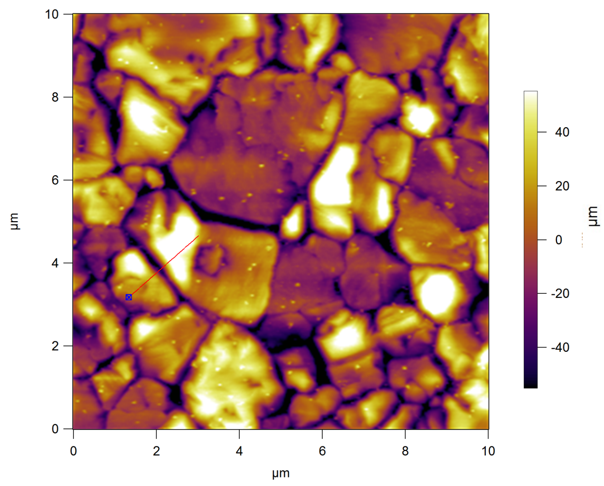


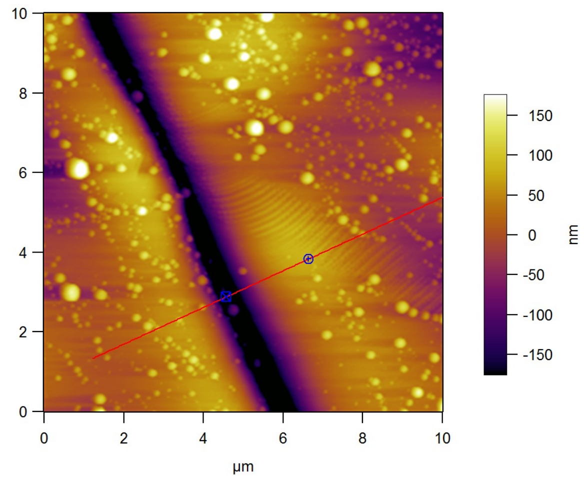




$$\bar{c}(z) \approx \bar{c}_{gb}(z) \propto \operatorname{erfc}\left(\frac{z}{2\sqrt{D_{gb}t}}\right)$$

Preliminary Dihedral Analysis

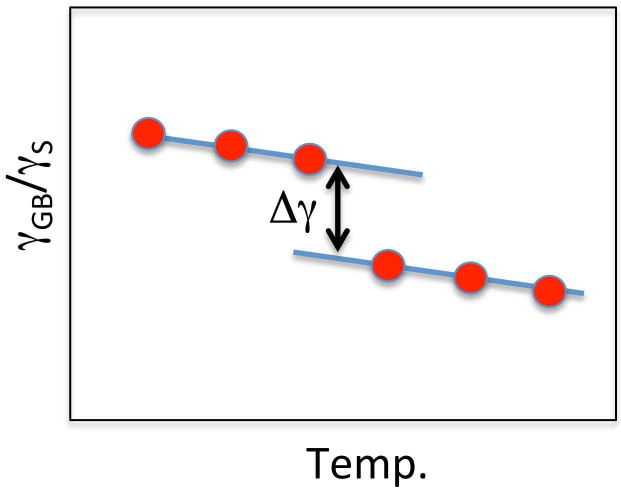


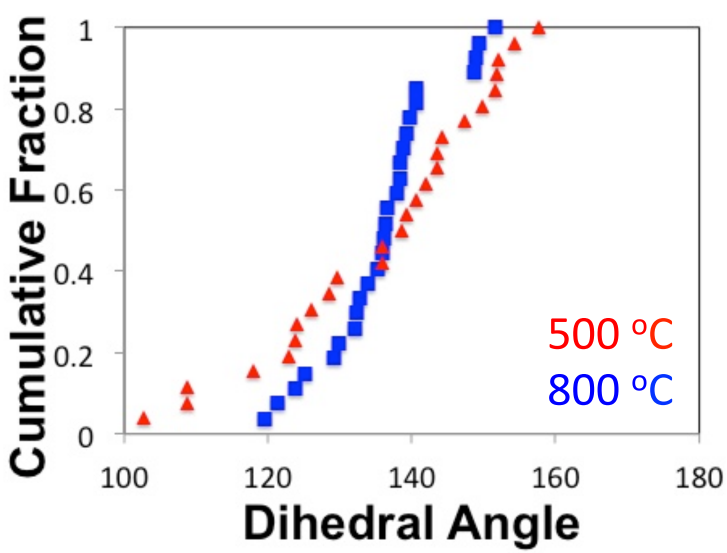


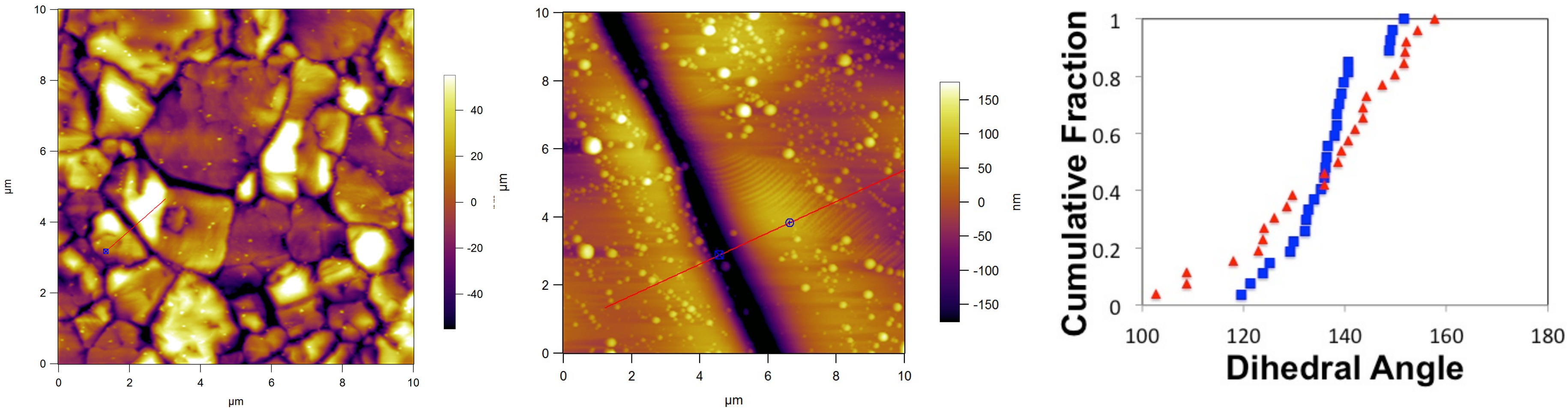
Measuring Δγ for:

$\Delta\gamma = \Delta\rho[-T(\Delta S_I - \Delta S_{II}) + (\Delta H_I - \Delta H_{II})]$

Expected data:







μm
μm
μm
μm
nm
Cumulative Fraction
Dihedral Angle

Equations for Fitting Diffusion Data

Type B

Instantaneous Source

$$sD_{gb}\delta = 1.322\sqrt{\frac{D}{t}}(-\partial\bar{c}/\partial z^{6/5})^{-5/3}$$

Constant Source

$$sD_{gb}\delta = 1.308\sqrt{\frac{D}{t}}(-\partial\bar{c}/\partial z^{6/5})^{-5/3}$$

Type C

Instantaneous Source

$$\bar{c}(z) \approx \bar{c}_{gb}(z) \propto \exp\left(-\frac{z^2}{4D_{gb}t}\right)$$

Constant Source

$$\bar{c}(z) \approx \bar{c}_{gb}(z) \propto \operatorname{erfc}\left(\frac{z}{2\sqrt{D_{gb}t}}\right)$$

Mobile Grain Boundaries

$$\delta D_{\mathrm{b}} = v\left(\frac{\partial \ln \bar{c}}{\partial z}\right)^{-2}$$