Modeling on Diffusion in Ni-base Superalloy

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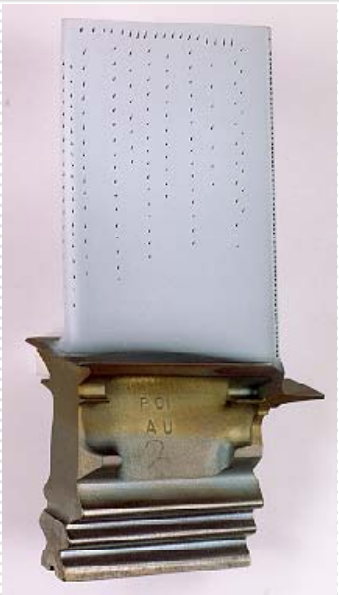
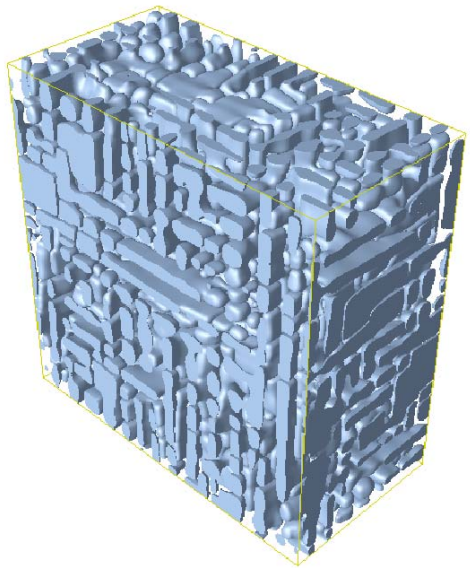
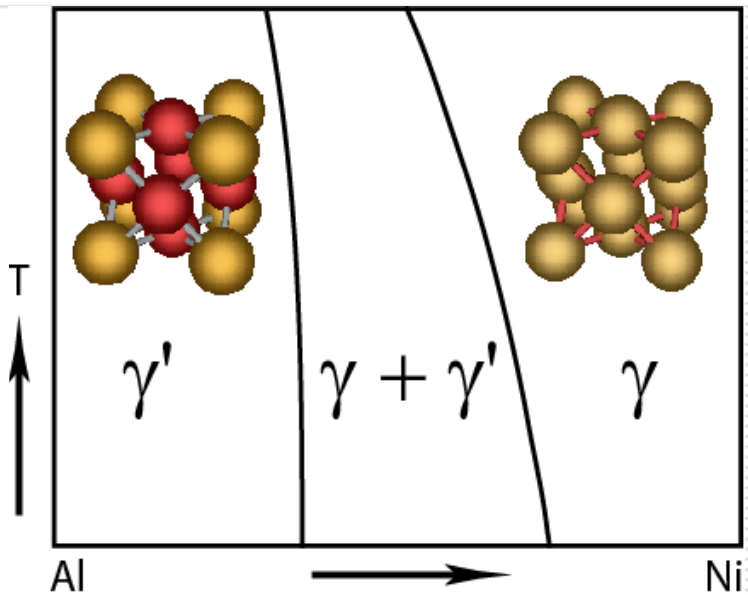
Microstructure Evolution of Ni-base Alloys

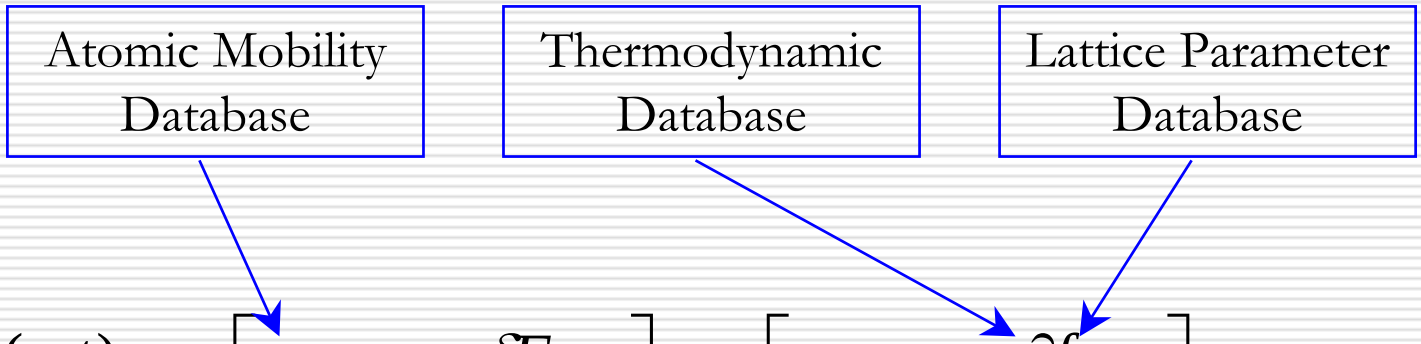






- A real turbine blade made of Ni-base superalloys, a γ (fcc) and γ' ($L1_2$) two phase microstructure from a phase-field simulation, and a schematic phase diagram for the γ and γ' two-phase field.

Evolution Equations in Phase-field Model



$$\frac{\partial c_i(\mathbf{r},t)}{\partial t} = \nabla\left[M_{im} \nabla \frac{\delta F}{\delta c_m(\mathbf{r},t)} \right] = \nabla\left[M_{im} \nabla \frac{\partial f}{\partial c_m(\mathbf{r},t)} \right]$$

$$\frac{\partial \phi_j(\mathbf{r},t)}{\partial t} = -L_{jn} \frac{\delta F}{\delta \phi_n(\mathbf{r},t)} = -L_{jn}\left(\varepsilon^2 \nabla^2 \phi_n(\mathbf{r},t) - \frac{\partial f}{\partial \phi_n(\mathbf{r},t)} \right)$$

- M is diffusion mobility and L is phase field mobility.

Modeling on Atomic Mobility

$$M_i = \frac{M_i^0}{RT}\exp(\frac{-Q_i}{RT}) = \frac{1}{RT}\exp(\frac{-Q_i + RT\ln M_i^0}{RT})$$

$$M_i = \frac{1}{RT}\exp(\frac{-\Delta G_i}{RT})$$

$$\Delta G_i = \sum_l x_l \Delta G_i^l + \sum_j \sum_{k>j} x_j x_k \Delta G_i^{j,k}$$

A-B binary system:

$$M = x_A x_B \left(x_A M_B + x_B M_A\right)$$

M: diffusion mobility in phase field

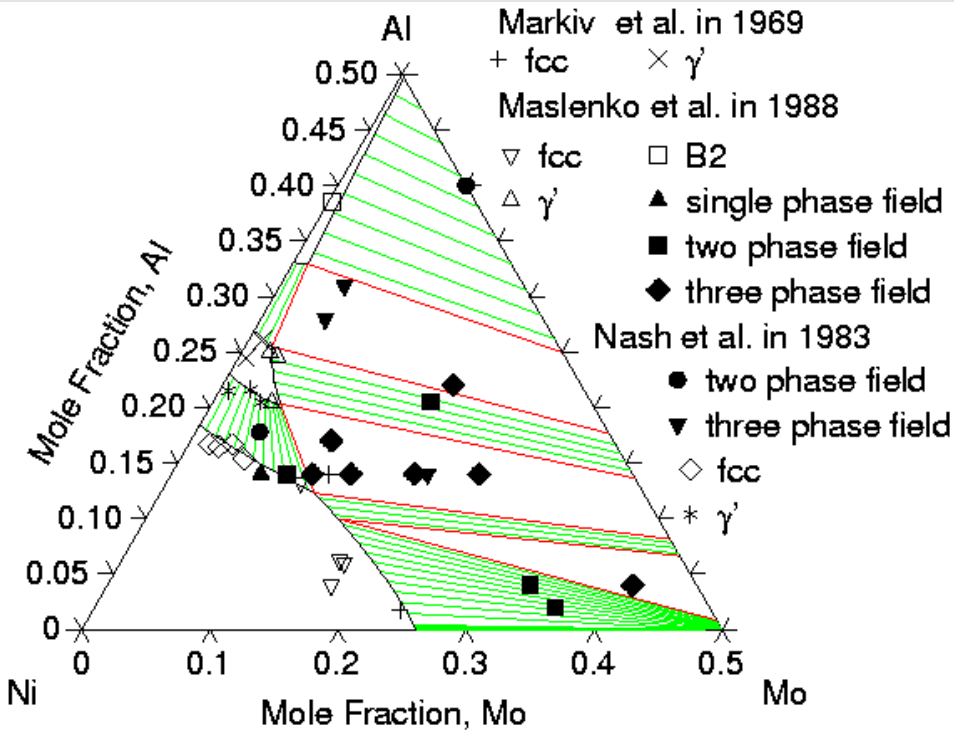
- Ordered Phases:

$$\Delta G_i = \Delta G_i^{dis} + \Delta G_i^{ord}$$

$$\Delta G_i^{ord} = \sum_j \sum_{k\neq j} \Delta G_{ijk}^{order} [y_j^\alpha y_k^\beta - x_j x_k]$$

- Andersson J and Agren J, J Appl Phys, 72 (1992) 1350
- Helander T and Agren J, Acta Mater, 47 (1999) 1141

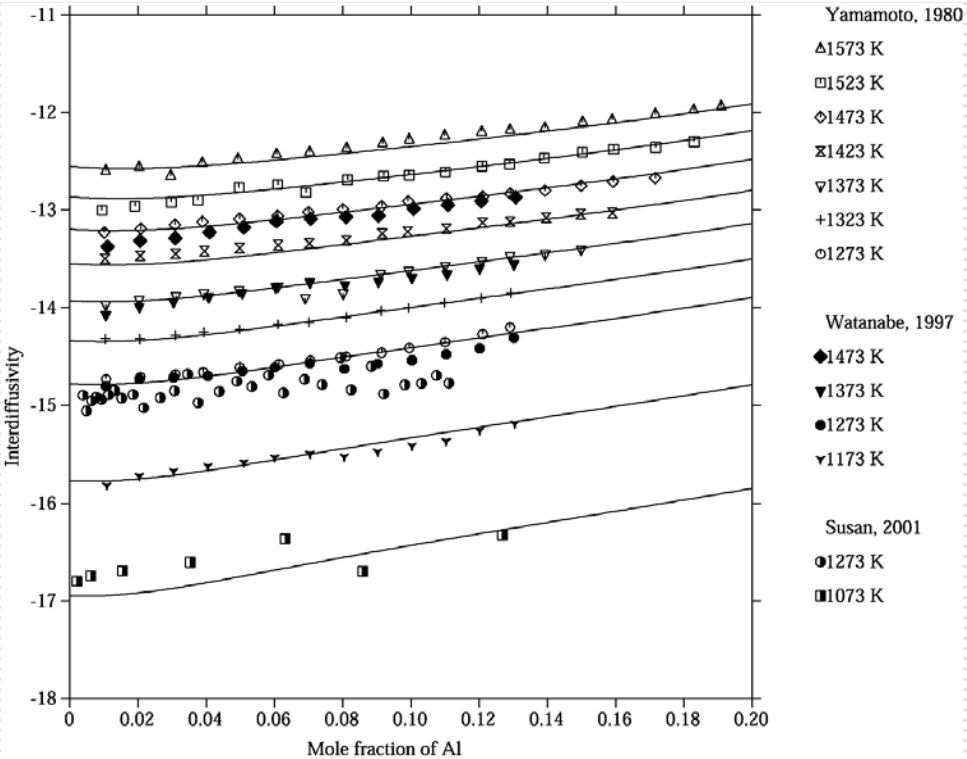
Thermodynamic Database



- 1473K

- *S. Zhou et al., in submission, (2005)*

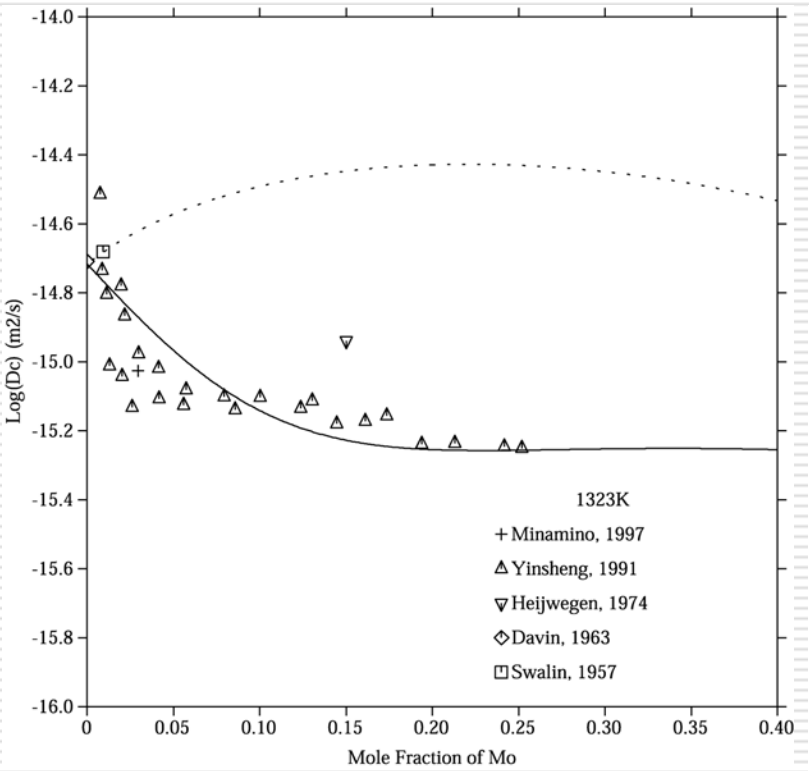
Diffusivity in Ni-Al fcc Phase



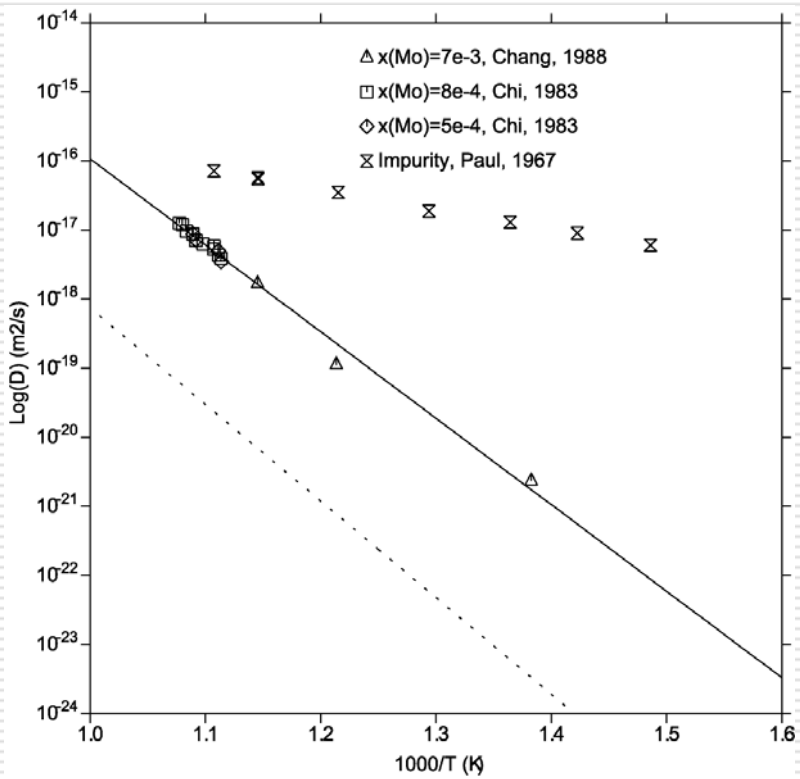
- Ni-Al

- *A. Engstrom, J. Agren, Z.Metallkd., 97 (1996) 92*

Diffusivity in fcc Phase

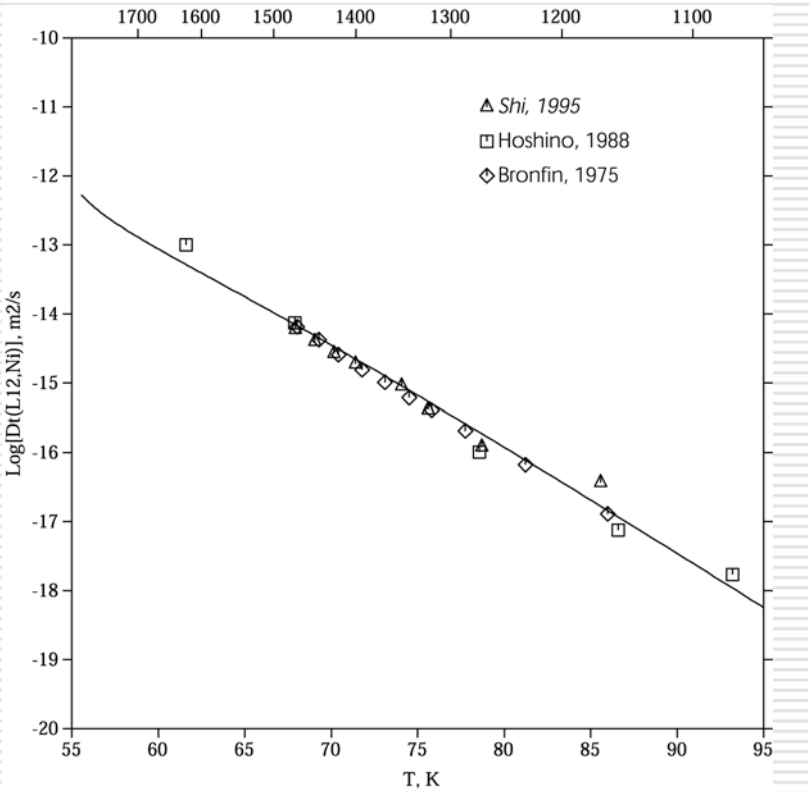


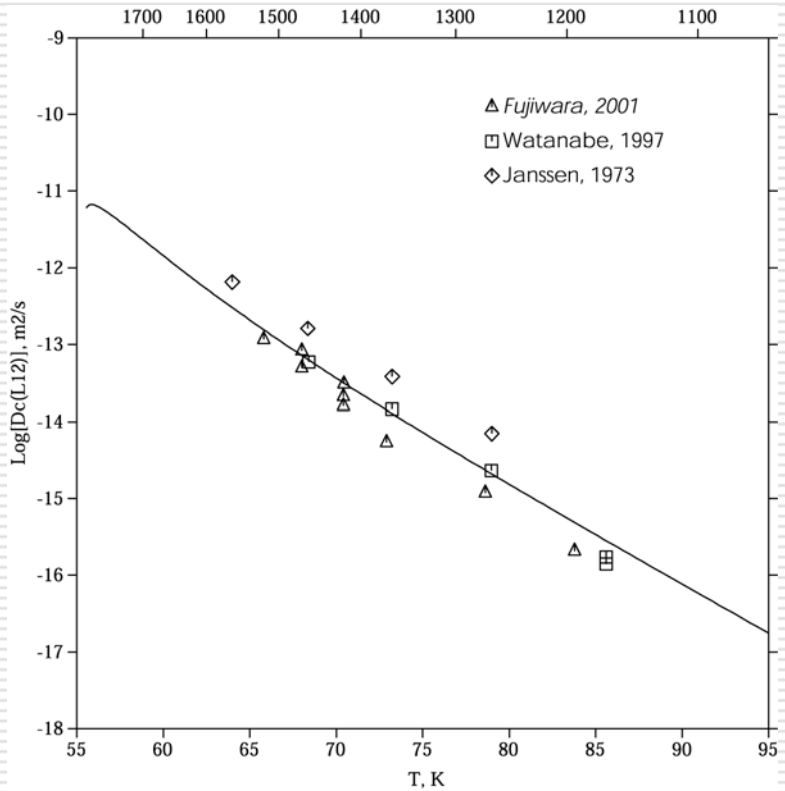
- Ni-Mo



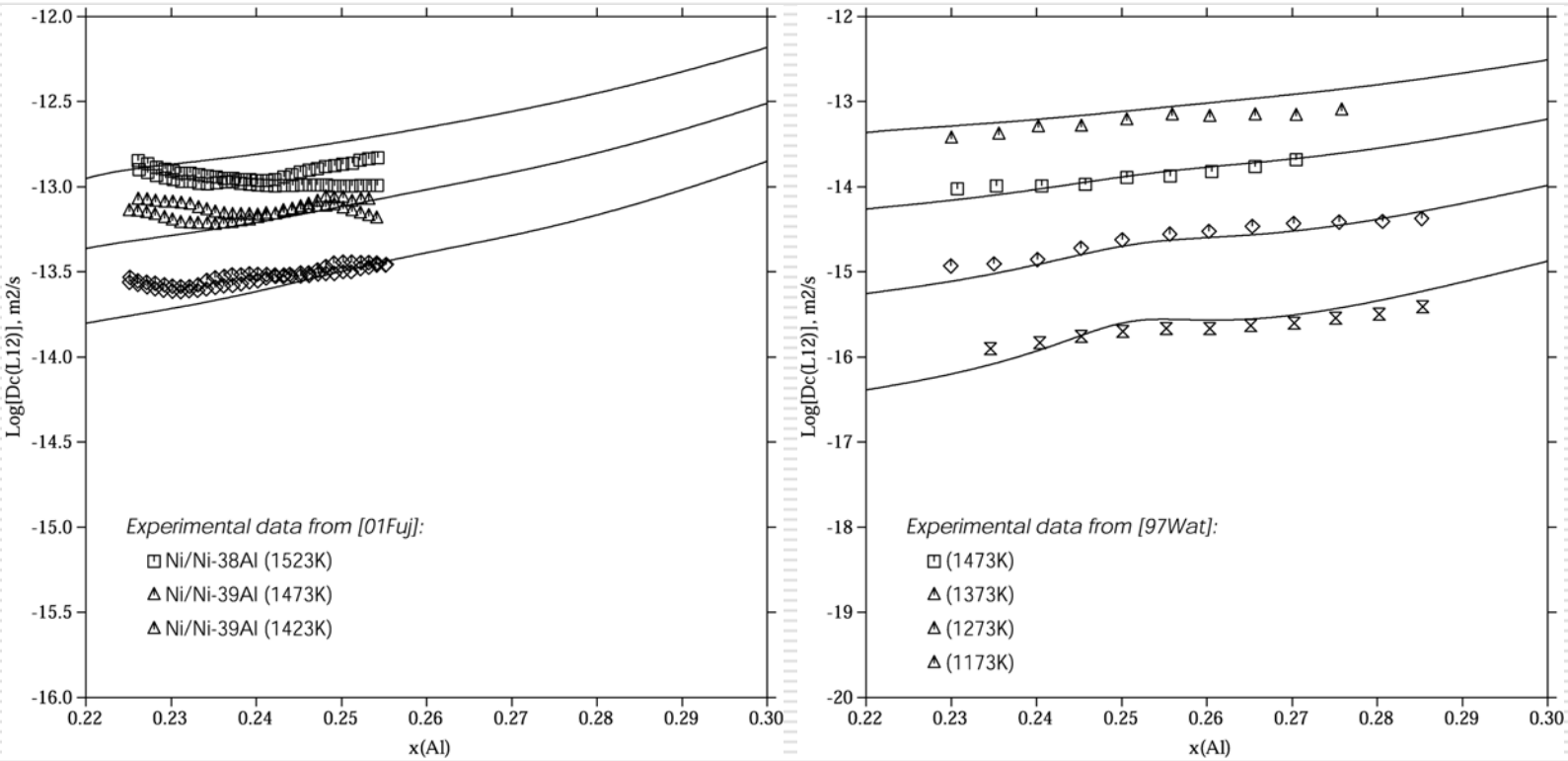
- Al-Mo

Diffusivity in Stoichiometric Compound (Assessment I)

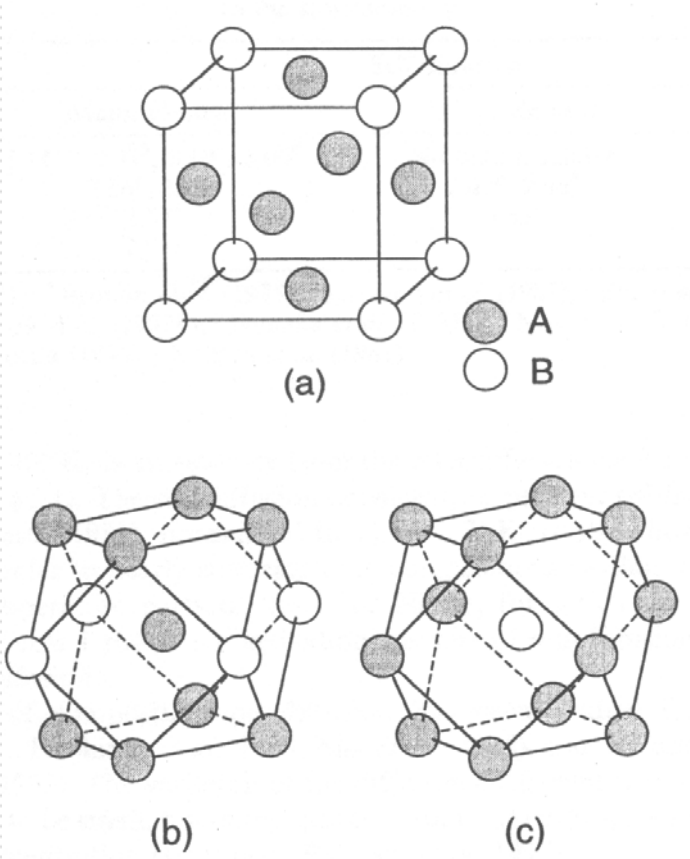




Diffusivity vs Composition (Assessment I)

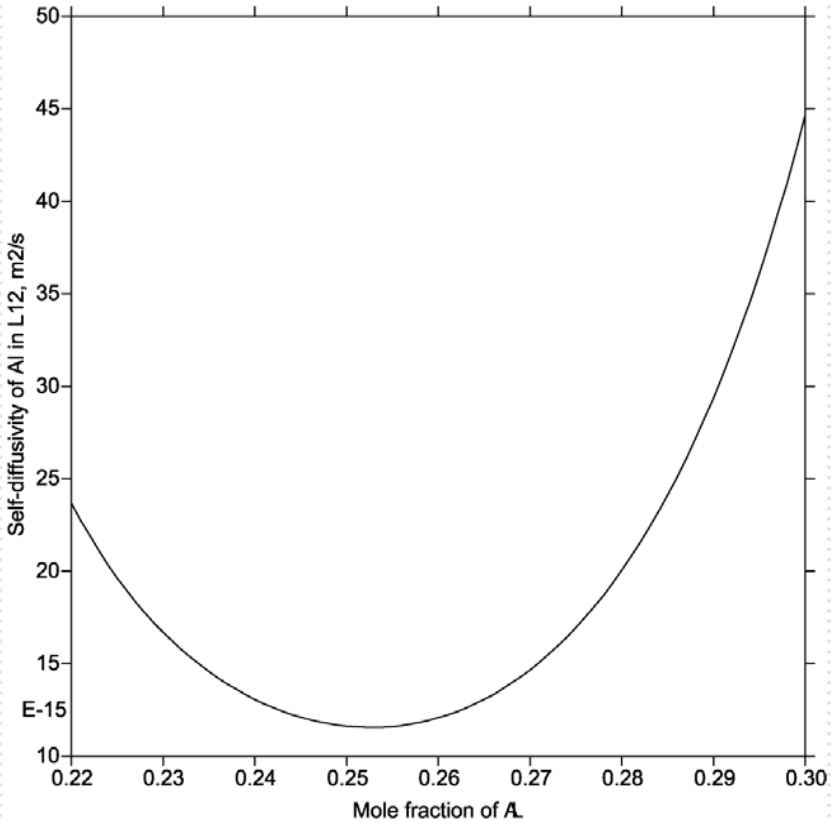


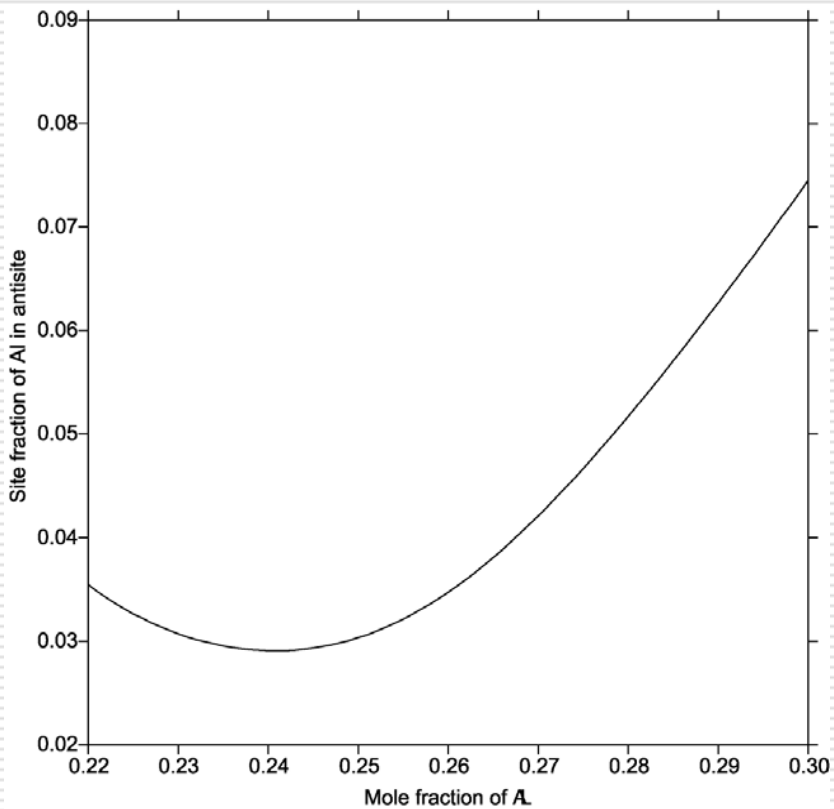
Diffusion Mechanism in $L1_2$



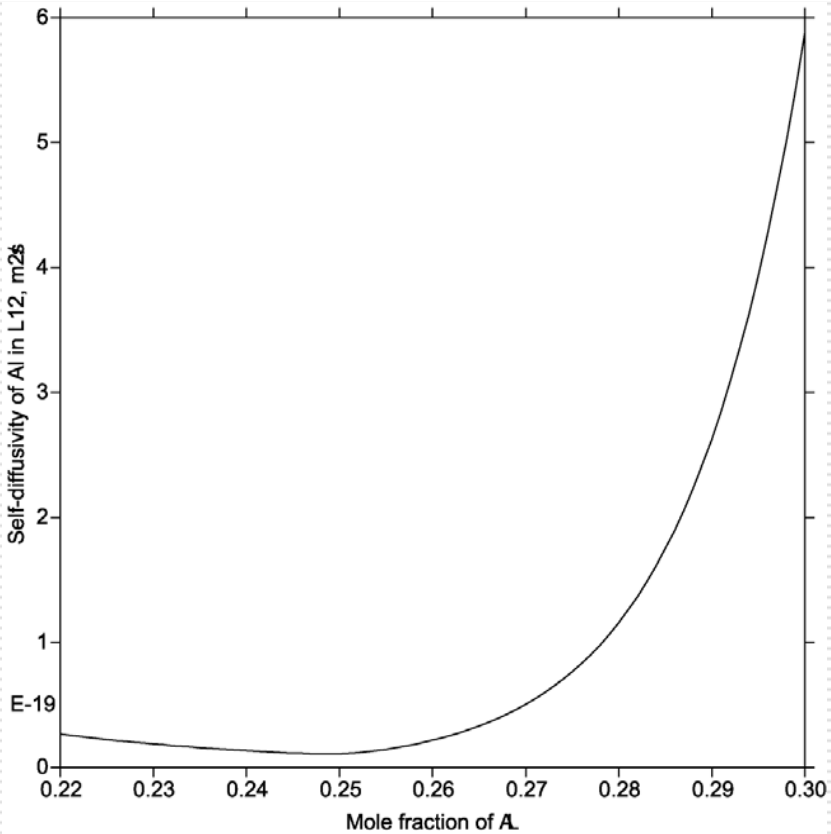
- Major element (Ni)
  - *intra-lattice mechanism*
- Minor element (Al)
  - *six-jump cycle mechanism*
  - *anti-site mechanism*
  - *anti-site bridge mechanism*

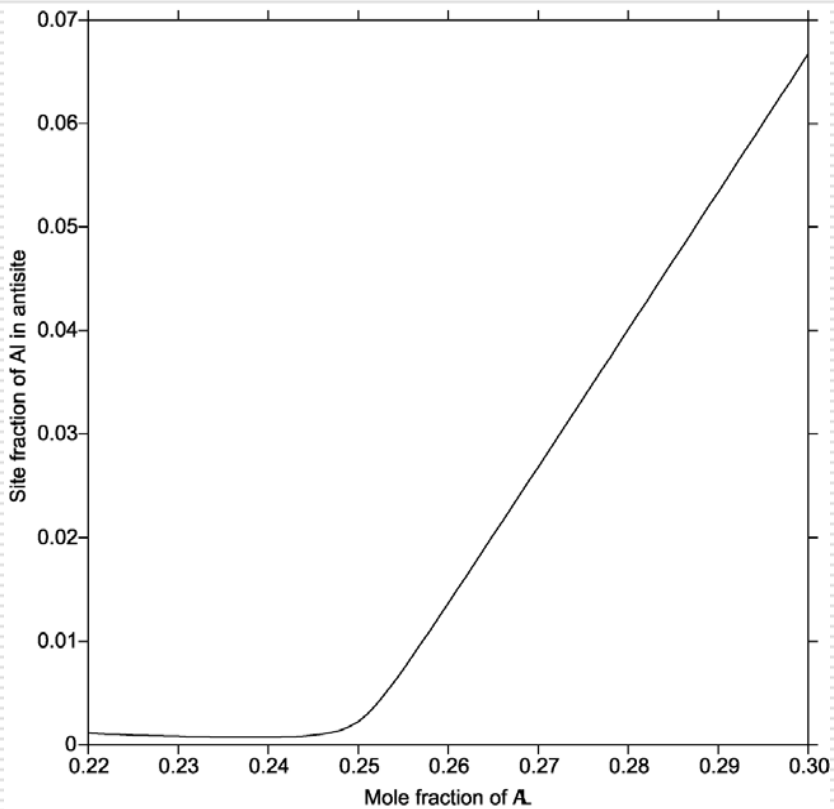
Diffusivity of Al (1473K)





Diffusivity of Al (973K)





Atomic Description for Diffusivity

- Ni in the fcc Ni Matrix:

$$D_{Ni}^{Ni} = a_{Ni}^{2} C_V^{Ni} \omega_0^{Ni} f^{Ni}$$

- Ni in the Ni3Al Matrix:

$$D_{Ni}^{Ni_3Al} = \frac{2}{3} a_{Ni_3Al}^{2} C_V^{Ni_3Al} \omega_0^{Ni_3Al} f^{Ni_3Al}$$

- Al in the fcc Ni Matrix:

$$D_{Al}^{Ni} = a_{Ni}^{2} C_V^{Ni} \frac{\omega_4^{Ni}}{\omega_3^{Ni}} \omega_2^{Ni} f^{Ni}$$

- Al in the Ni3Al Matrix:

$$D_{Al}^{Ni_3Al} = \frac{2}{3} a_{Ni_3Al}^{2} C_V^{Ni_3Al} \frac{\omega_4^{Ni_3Al}}{\omega_3^{Ni_3Al}} \omega_2^{Ni_3Al} f^{Ni_3Al} P_{Al}^{Ni}$$

Numerical Treatment

- P_{Al}^{Ni} : anti-site factor.

$$P_{Al}^{Ni} = \frac{y_{Al}^{Ni}}{x_{Al}}$$

- $(\omega_4 / \omega_3)(\omega_2 / \omega_0)$: reflects the impurity-vacancy and impurity-matrix interactions, assumed to be equal for the diffusion of Al in Ni_3Al and fcc Ni.

$$\frac{D_{Al}^{Ni_3Al}}{D_{Al}^{Ni}} \frac{D_{Ni}^{Ni}}{D_{Ni}^{Ni_3Al}} \approx P_{Al}^{Ni}$$

- *H. Numakura, et al., Phil. Mag. A, 77 (1998) 887*

Dictra Modeling on Diffusivity

- Ni in the fcc Ni Matrix:

$$D_{Ni}^{dis} = \exp\left(\frac{-\Delta G_{Ni}^{dis}}{RT}\right)$$

- Ni in the Ni_3Al Matrix:

$$D_{Ni}^{Ni_3Al} = \exp\left(-\frac{\Delta G_{Ni}^{dis} + \Delta G_{Ni}^{ord}}{RT}\right)$$

- Al in the fcc Ni Matrix:

$$D_{Al}^{dis} = \exp\left(\frac{-\Delta G_{Al}^{dis}}{RT}\right)$$

- Al in the Ni_3Al Matrix:

$$D_{Al}^{Ni_3Al} = \exp\left(-\frac{\Delta G_{Al}^{dis} + \Delta G_{Al}^{ord}}{RT}\right)$$

Numerical Treatment II

$$\frac{D_{Al}^{Ni_3Al}}{D_{Al}^{Ni}}\frac{D_{Ni}^{Ni}}{D_{Ni}^{Ni_3Al}} = \exp\left(-\frac{\Delta G_{Al}^{ord} - \Delta G_{Ni}^{ord} + \Delta G'}{RT}\right)$$

- Where $\Delta G' = \Delta G_{Al}^{dis} + \Delta G_{Ni}^{Ni} - \Delta G_{Al}^{Ni} - \Delta G_{Ni}^{dis}$, which can be calculated from the mobility descriptions of the related disordered phase.

Constraint from Diffusion Mechanism

$$\frac{D_{Al}^{Ni_3Al}}{D_{Al}^{Ni}}\frac{D_{Ni}^{Ni}}{D_{Ni}^{Ni_3Al}} = P_{Al}^{Ni}$$

$$\frac{D_{Al}^{Ni_3Al}}{D_{Al}^{Ni}}\frac{D_{Ni}^{Ni}}{D_{Ni}^{Ni_3Al}} = \exp\left(-\frac{\Delta G_{Al}^{ord} - \Delta G_{Ni}^{ord} + \Delta G'}{RT}\right)$$

$$\Downarrow$$

$$\exp\left(-\frac{\Delta G_{Al}^{ord} - \Delta G_{Ni}^{ord} + \Delta G'}{RT}\right) = P_{Al}^{Ni}$$

Anti-site Factor

- Consider reaction:

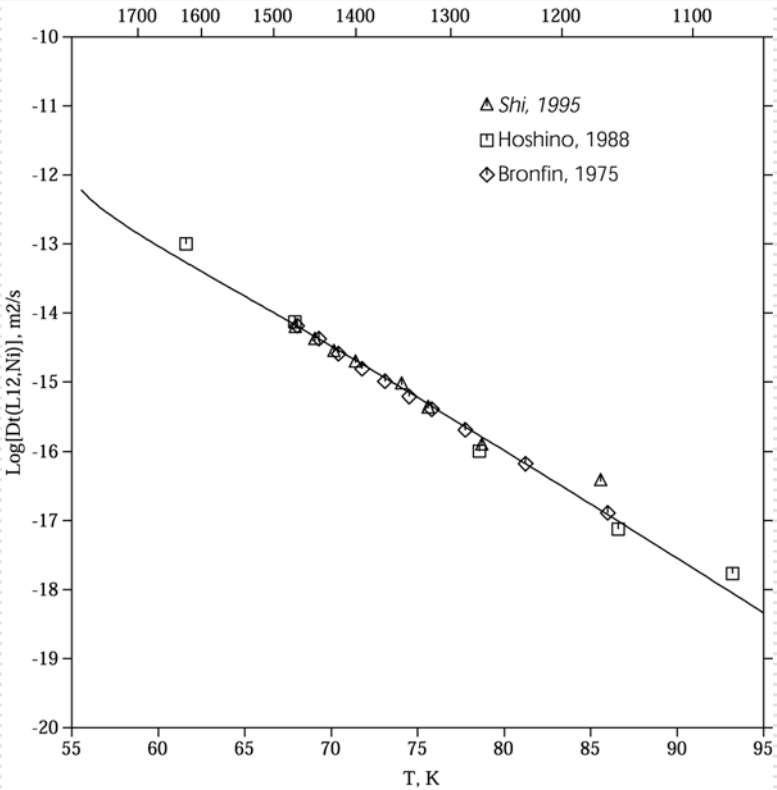
$$Ni_3Al\,(L1_2) \leftrightarrow (Ni_{0.75}Al_{0.25})_3(Ni_{0.75}Al_{0.25})\,(fcc)$$

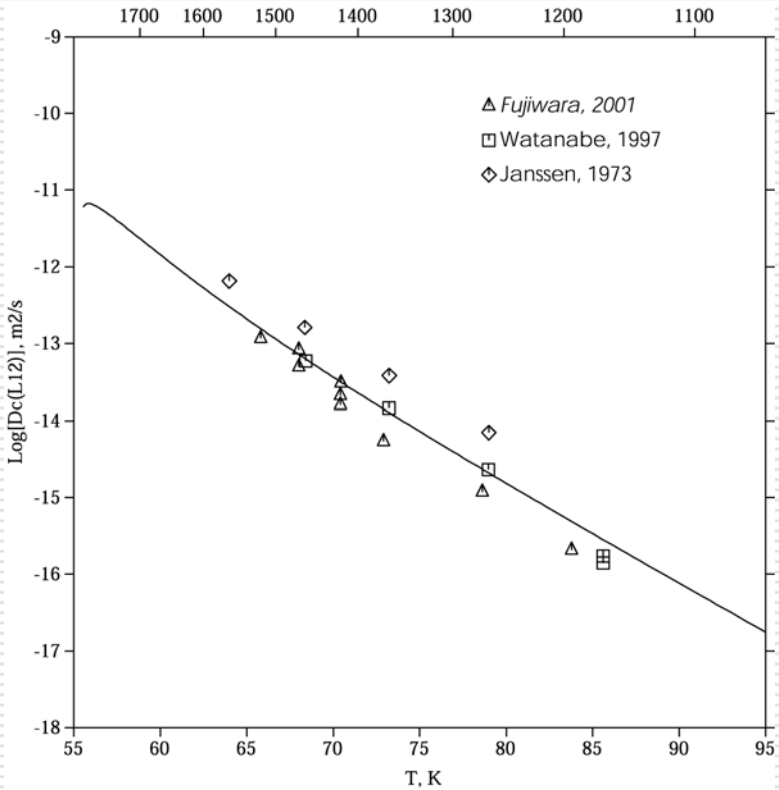
- Anti-site factor:

$$P_{Al}^{Ni} = \frac{y_{Al}^{Ni}}{x_{Al}} \approx f_{fcc} \approx \exp(-\frac{\Delta G^{react}}{RT})$$

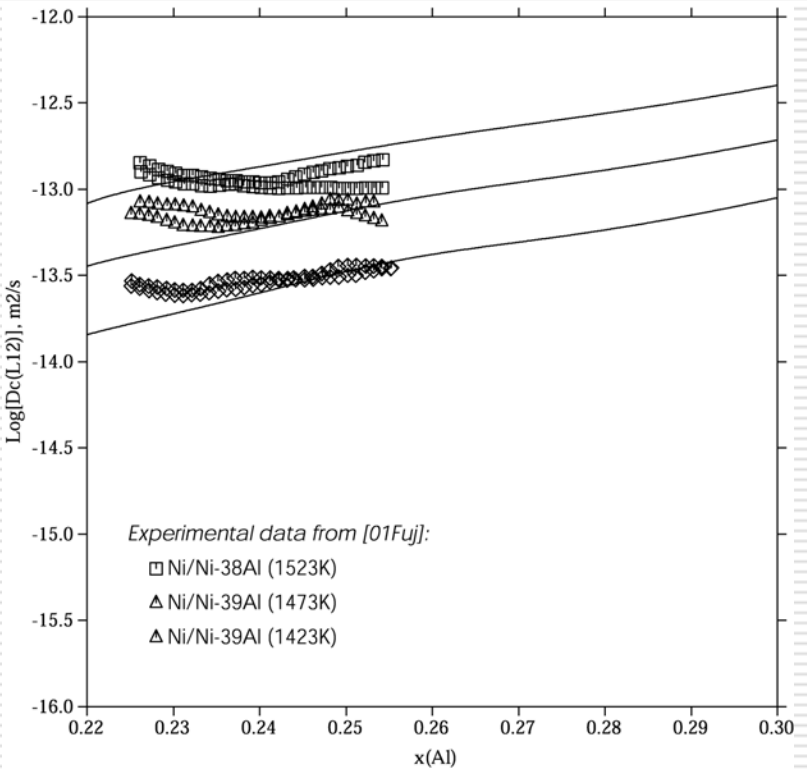
$$\Delta G_{Al}^{ord} - \Delta G_{Ni}^{ord} + \Delta G' = \Delta G^{react}$$

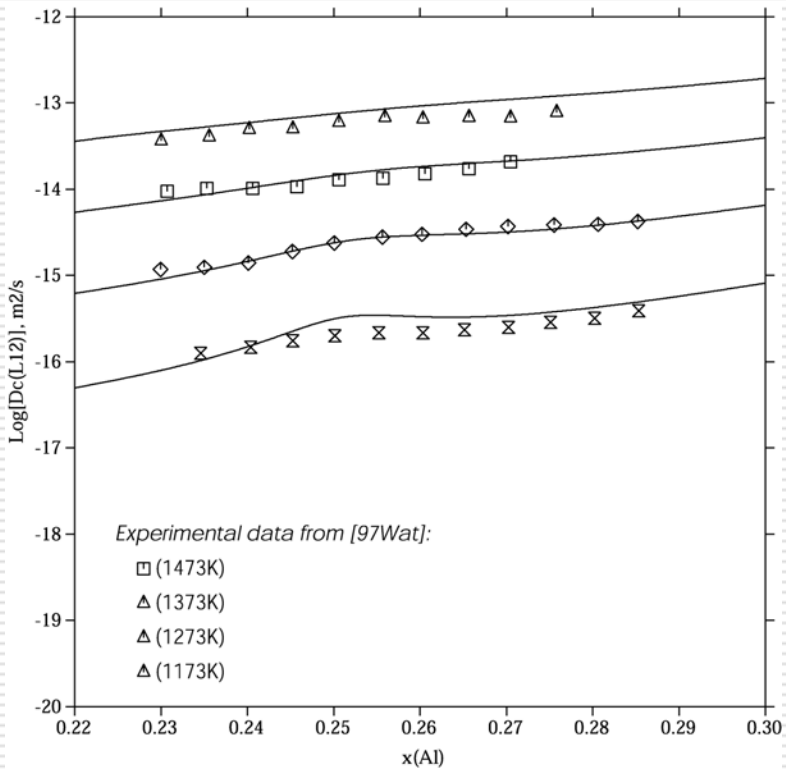
Diffusivity in Stoichiometric Compound (Assessment II)





Diffusivity vs Composition (Assessment II)





Optimized Parameters for Ni_3Al

	ΔG^{ord}_{AlNiAl}	ΔG^{ord}_{NiNiAl}	ΔG^{ord}_{AlAlNi}	ΔG^{ord}_{NiAlNi}
Assessment I	1.8804e+05	-9.3253e+04	6.0418e+05	-5.8868e+05
Assessment II	1.2499e+05	-7.8982e+04	3.6406e+05	-5.3770e+05

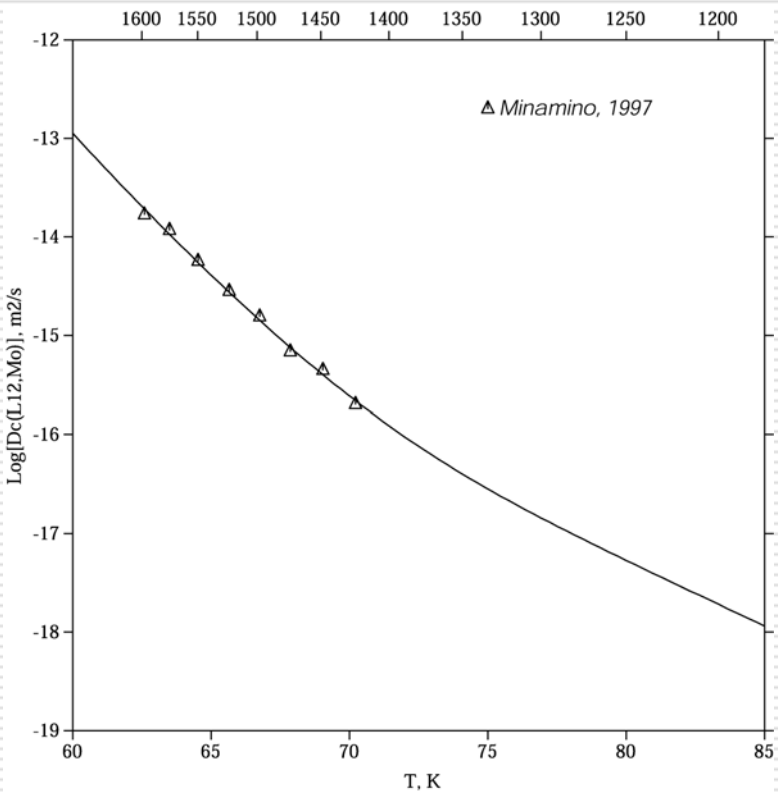
- Units: J/mole

Diffusion in $L1_2$ of the Ni-Al-Mo System

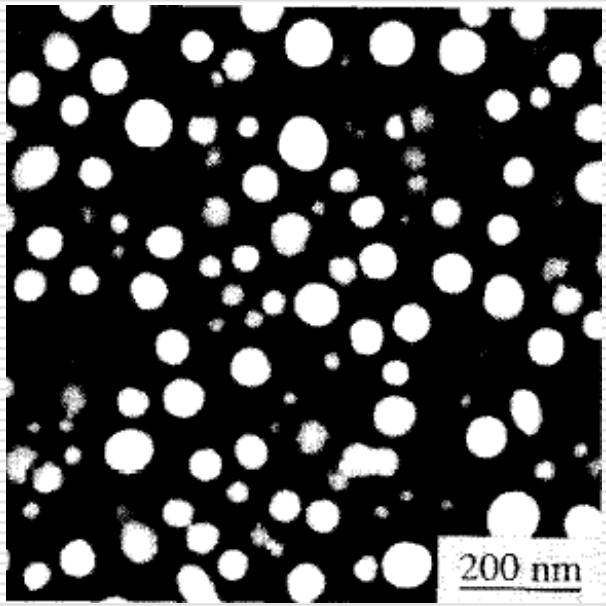
Since Mo prefers to occupy Al-sites in Ni_3Al ordered phase, we assume:

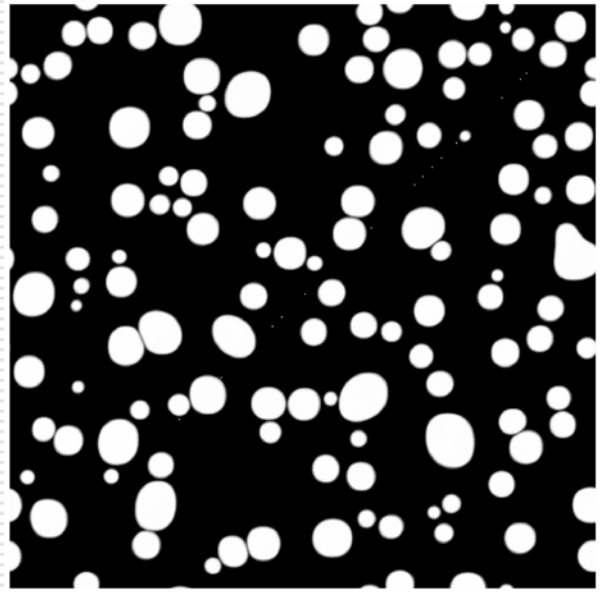
- The effect of Al-Mo ordering can be ignored.
- The diffusion in the hypothetical Ni_3Mo $L1_2$ ordered phase is similar to that in the Ni_3Al phase.
- The diffusion of Mo in the $L1_2$ ordered phase is similar to that of Al.

Diffusivity of Mo in Ni_3Al



Phase Field Simulation vs Experimental Investigation





- Alloy: Ni-7.7 at.%Al-7.9 at.%Mo
- System size: 1024nm×1024nm; Temperature: 1048K; Annealing time: 67h
- Left: TEM images; Right: 2D phase-field simulations

Summary

- The atomic mobility modeling of Ni-Mo and Al-Mo fcc phases has been carried out based on the available experimental data. By combining them with previous work on Ni-Al, the mobility database for the fcc phase of the Ni-Al-Mo system has been developed.
- The effect of chemical ordering on atomic mobility is described by a phenomenological model. The available experimental data for Ni_3Al are used to evaluate the model parameters.
- The anti-site mechanism is found to be dominant for Al diffusion in $L1_2$. The atomic mobility modeling is then refined based on the anti-site mechanism.
- Atomic mobility in the $L1_2$ phase of Ni-Al-Mo system is evaluated from the experimental information in the literature.
- Using the above atomic mobility in the fcc and $L1_2$ phases, phase field simulations for Ni-Al-Mo alloys have been performed.