Diffusion in fcc and $L1_2$ Phases of Ni-Al-Mo

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Diffusion in the fcc Disordered Phase of the Ni-Al-Mo System

Modeling on Atomic Mobility

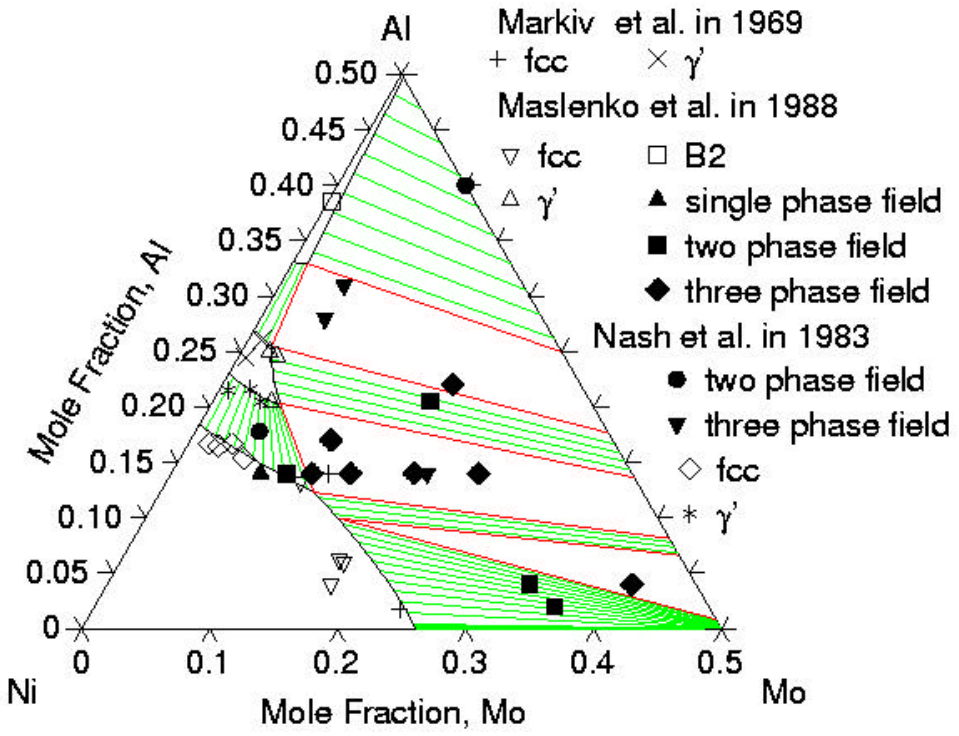
$$M_i = \frac{M_i^0}{RT}\exp(\frac{-Q_i}{RT}) = \frac{1}{RT}\exp(\frac{-Q_i + RT\ln M_i^0}{RT})$$

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

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

- *J. Andersson and J. Agren, J. Appl. Phys., 72 (1992) 1350*

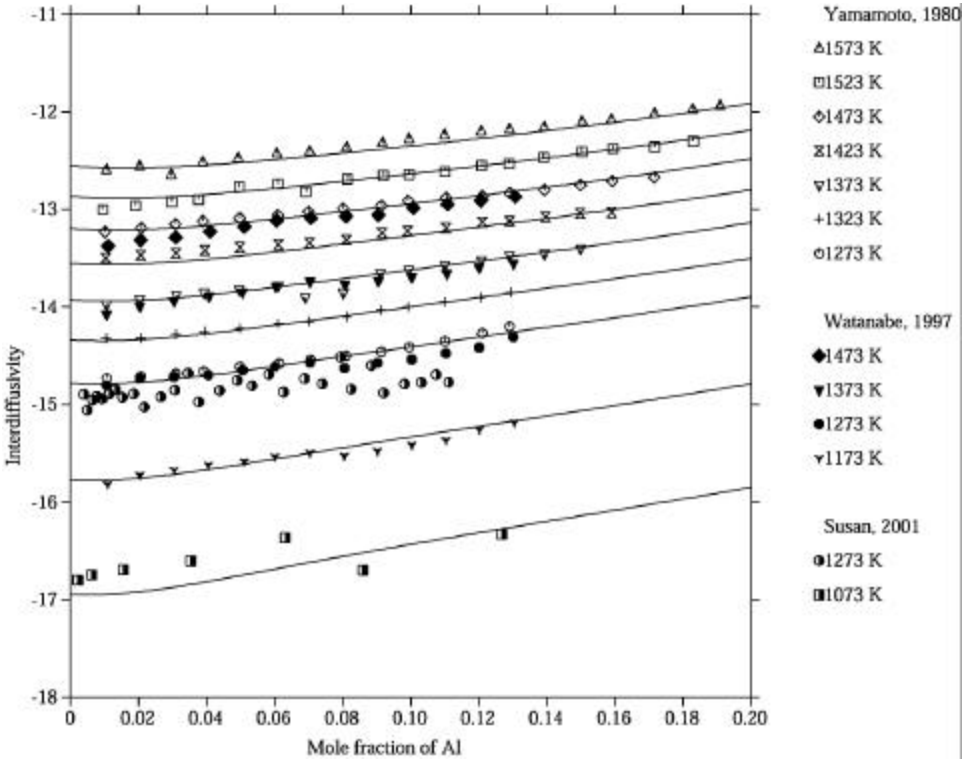
Thermodynamic Database



- 1473K

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

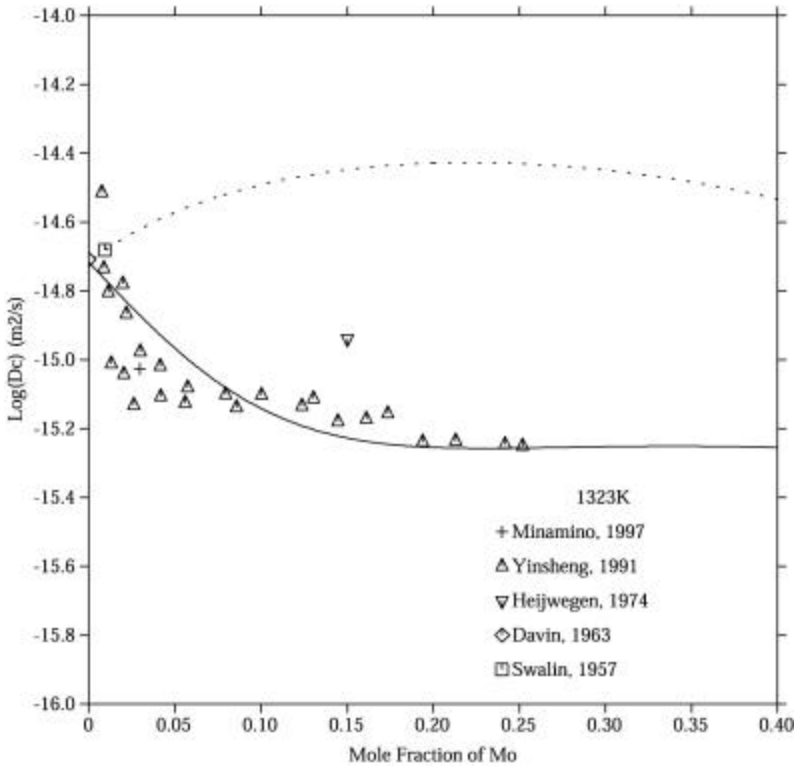
Diffusivity in Ni-Al fcc Phase



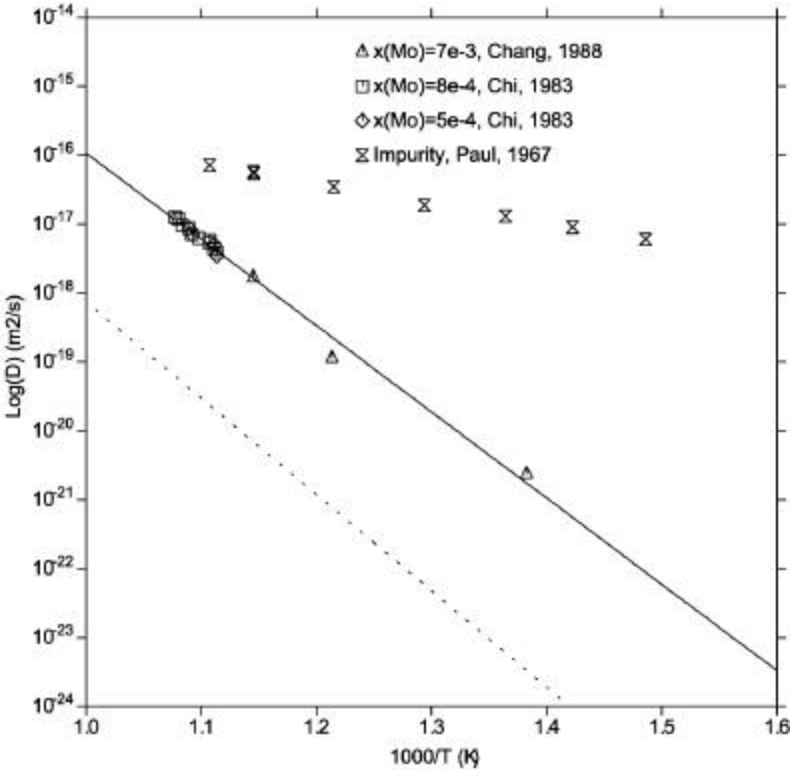
- Ni-Al

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

Diffusivity in fcc Phase



- Ni-Mo



- Al-Mo

Diffusion in the $L1_2$ Ordered Phase of the Ni-Al System

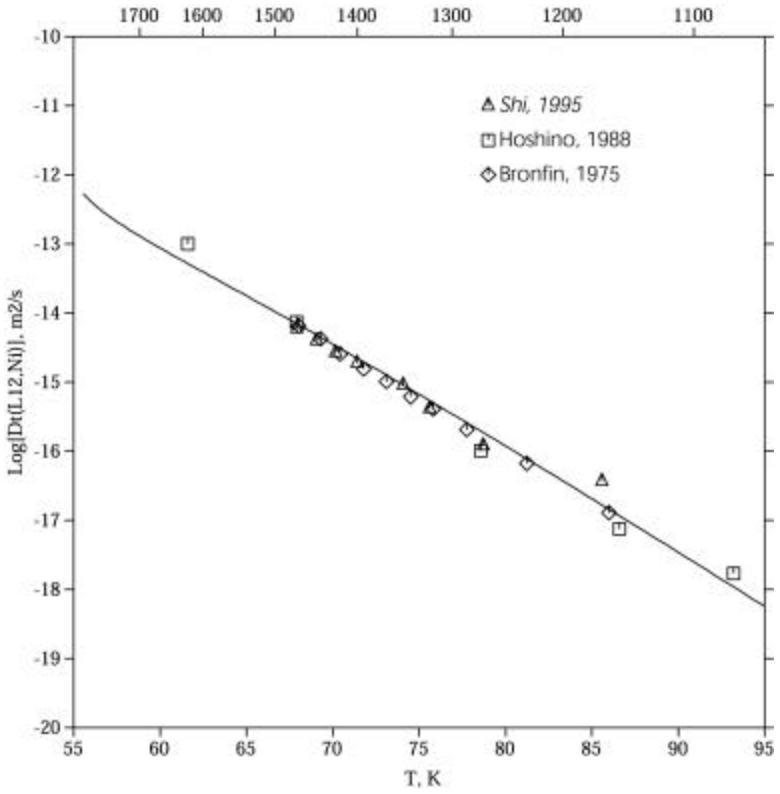
Modeling the Ordered Phase

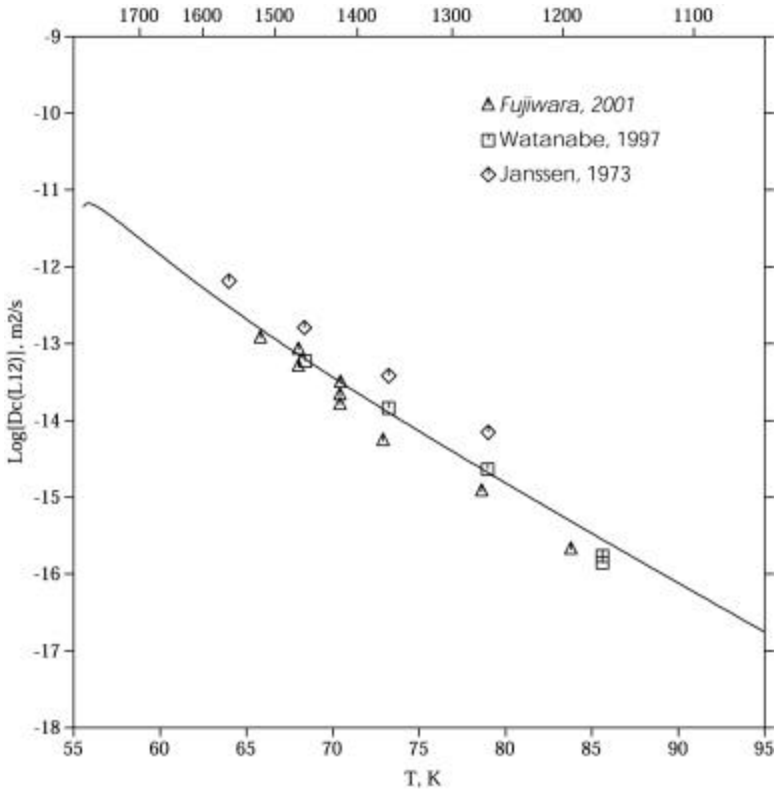
$$\Delta G_i = \Delta G_i^{dis} + \Delta G_i^{ord}$$

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

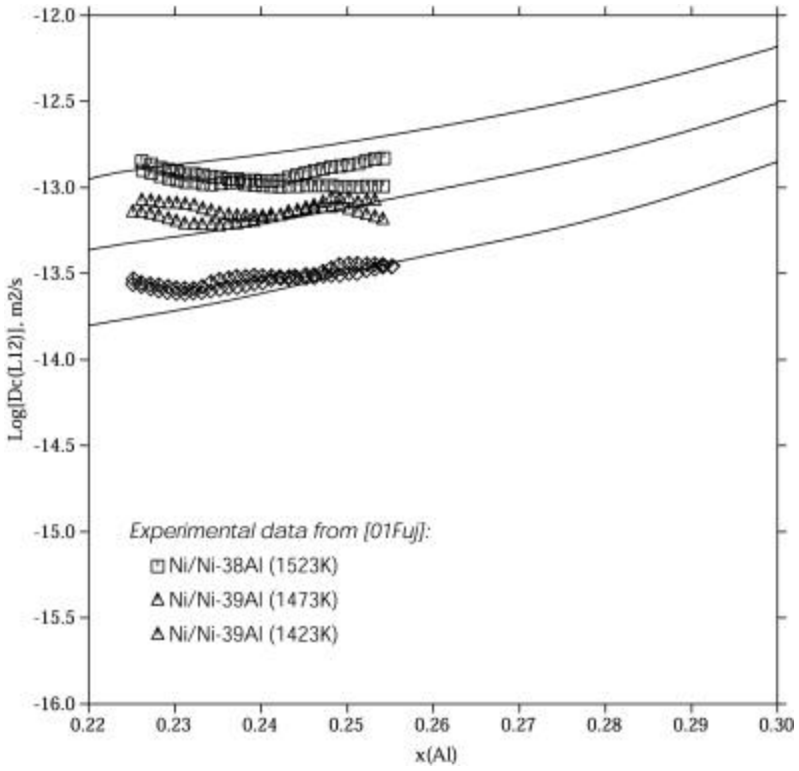
- *T. Helander and J. Agren, Acta Mater., 47 (1999) 1141*

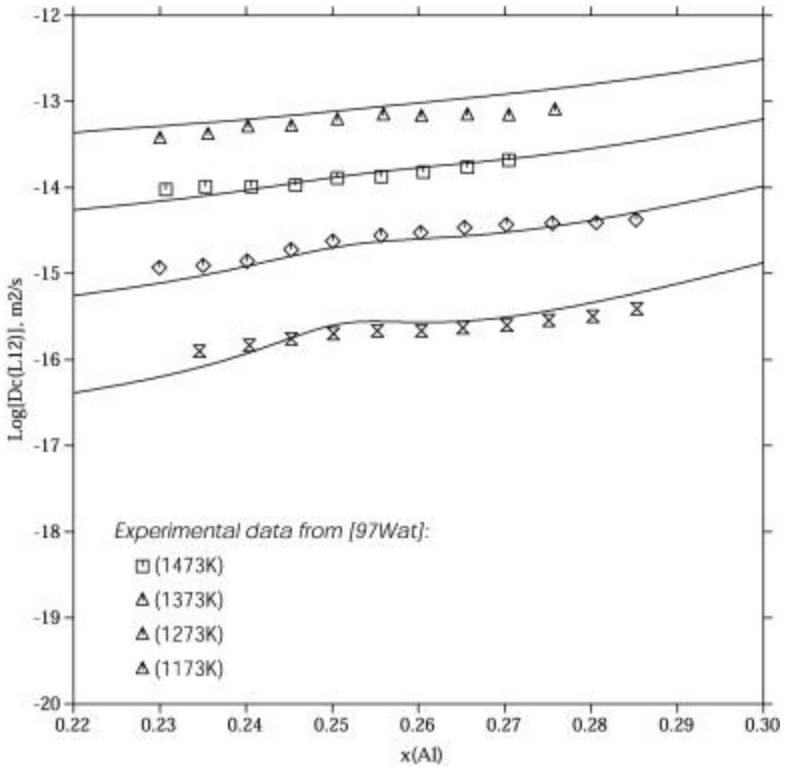
Diffusivity in Stoichiometric Compound (Assessment I)





Diffusivity vs Composition (Assessment I)

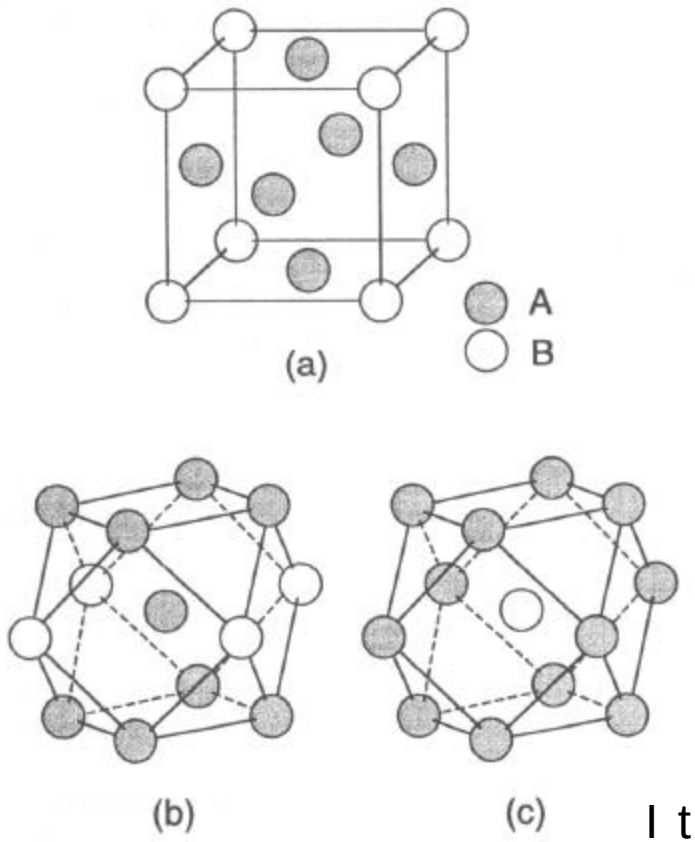




Diffusion in $L1_2$ Ordered Phase

The movements of vacancies should not destroy the ordered structure.

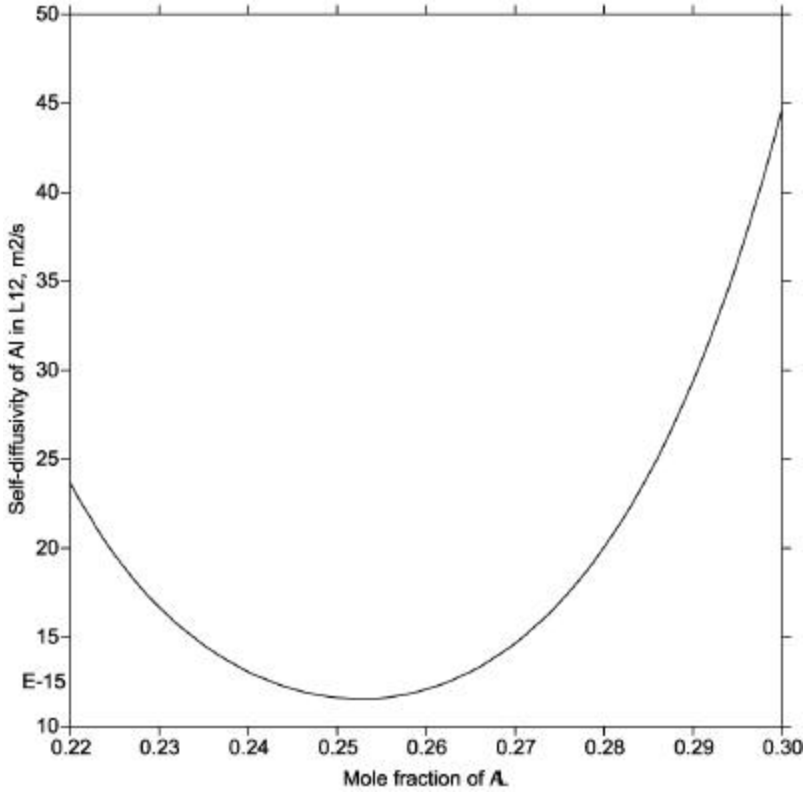
Diffusion Mechanism in $L1_2$

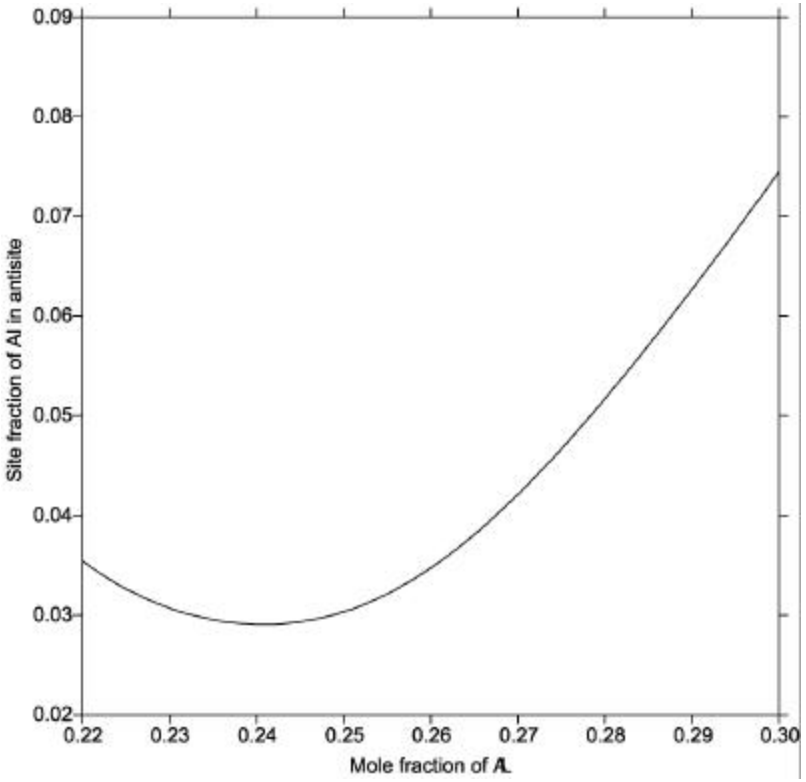


- Major element (Ni)
  - *intra-lattice mechanism*
- Minor element (Al)
  - *six-jump cycle mechanism*
  - *anti-site mechanism*
  - *anti-site bridge mechanism*

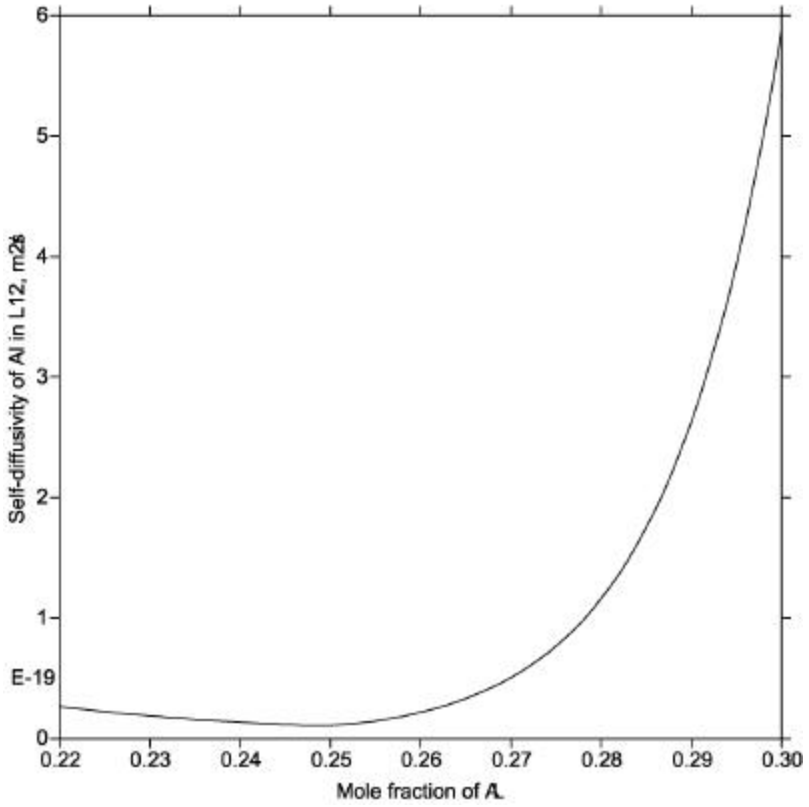
I think you need extra illustration to show the 3 mechanisms

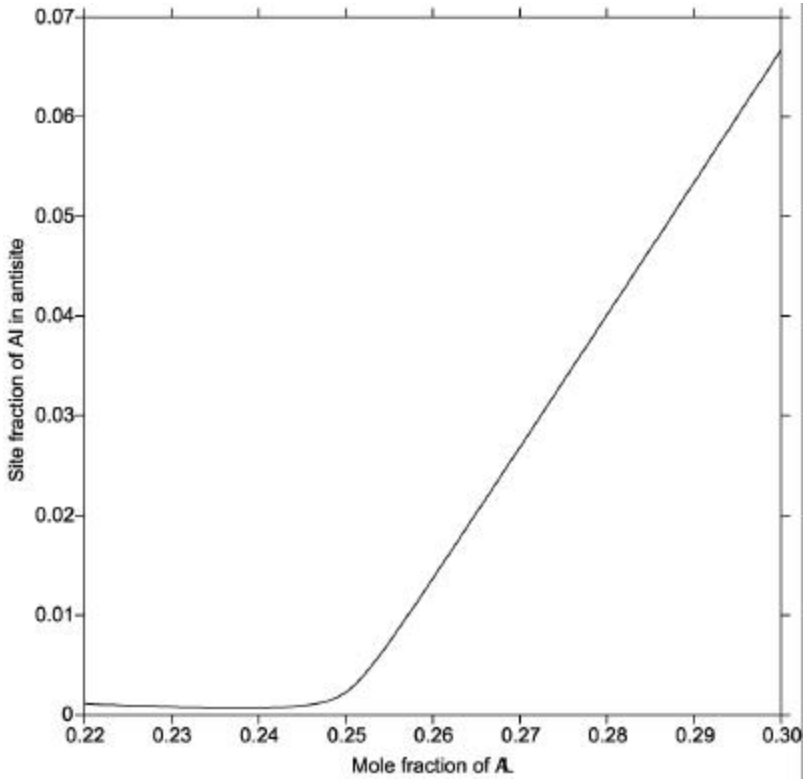
Diffusivity of Al (1473K)





Diffusivity of Al (973K)





Atomic Description for Diffusivity

- Ni in the fcc Ni Matrix:

$$D_{Ni}^{Ni} = a_{Ni}^{2} C_V^{Ni} w_0^{Ni} f^{Ni}$$

There is no explanation of ωo,ω1,ω2,ω3, etc.

- Ni in the Ni_3Al Matrix:

$$D_{Ni}^{Ni_3Al} = \frac{2}{3} a_{Ni_3Al}^{2} C_V^{Ni_3Al} w_0^{Ni_3Al} f^{Ni_3Al}$$

- Al in the fcc Ni Matrix:

$$D_{Al}^{Ni} = a_{Ni}^{2} C_V^{Ni} \frac{w_4^{Ni}}{w_3^{Ni}} w_2^{Ni} f^{Ni}$$

- Al in the Ni_3Al Matrix:

$$D_{Al}^{Ni_3Al} = \frac{2}{3} a_{Ni_3Al}^{2} C_V^{Ni_3Al} \frac{w_4^{Ni_3Al}}{w_3^{Ni_3Al}} w_2^{Ni_3Al} f^{Ni_3Al} P_{Al}^{Ni}$$

Numerical Treatment

- $(w_4 / w_3)(w_2 / w_0)$: reflects the impurity-vacancy and impurity-matrix interactions, assumed to be equal for the diffusion of Al in Ni_3Al and fcc Ni.

- P_{Al}^{Ni}: anti-site factor. $P_{Al}^{Ni} = \dfrac{y_{Al}^{Ni}}{x_{Al}}$

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

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

Dictra Modeling on Diffusivity

- Ni in the fcc Ni Matrix:

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

- Ni in the Ni_3Al Matrix:

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

- Al in the fcc Ni Matrix:

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

- Al in the Ni_3Al Matrix:

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

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:

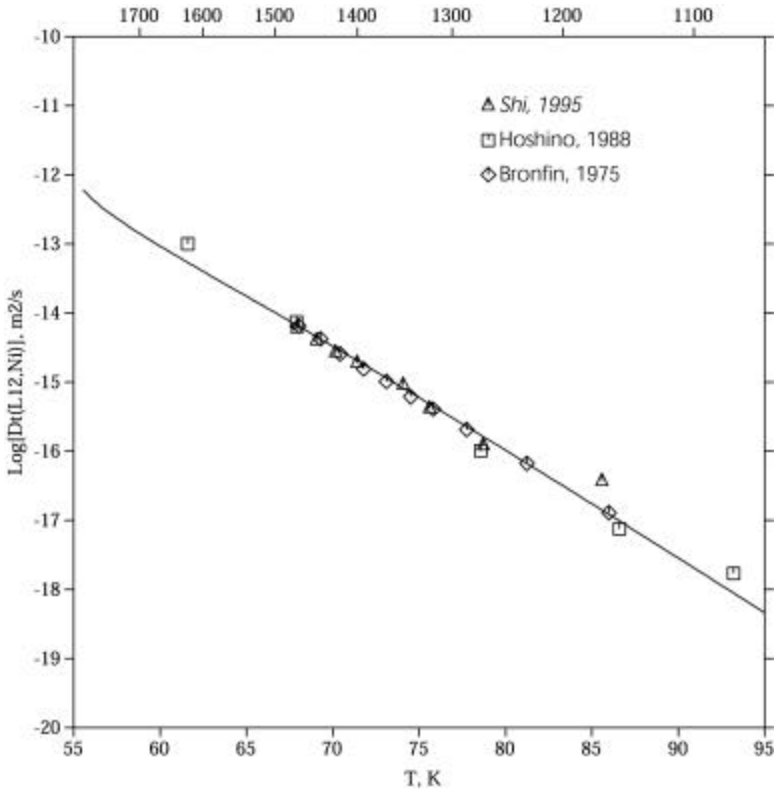
$$Ni_3Al\,(L1_2) \leftrightarrow (Ni_{0.75}Al_{0.25})_3(Ni_{0.75}Al_{0.25})\,(fcc)$$

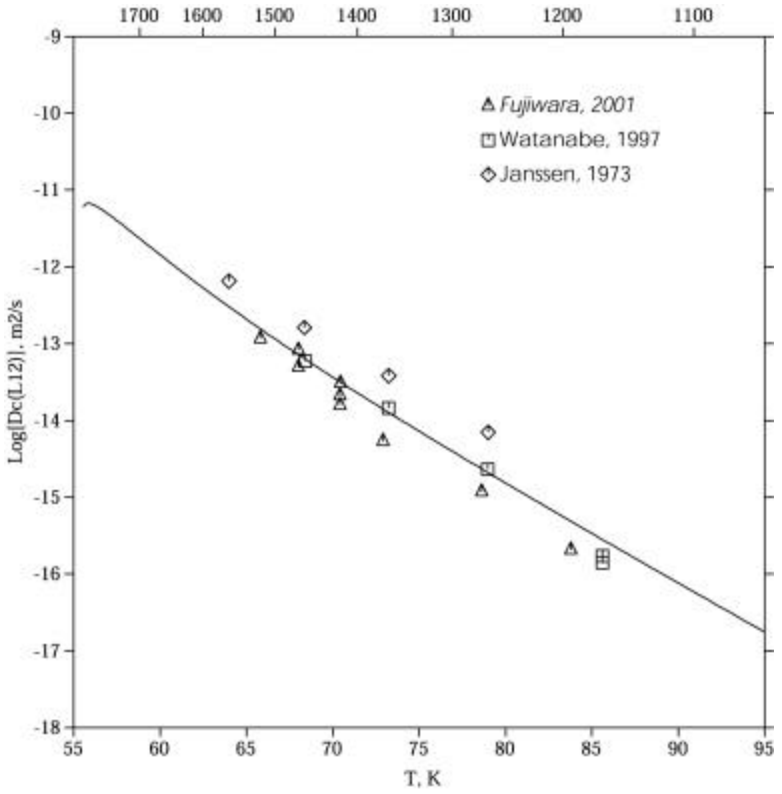
- Anti-site factor:

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

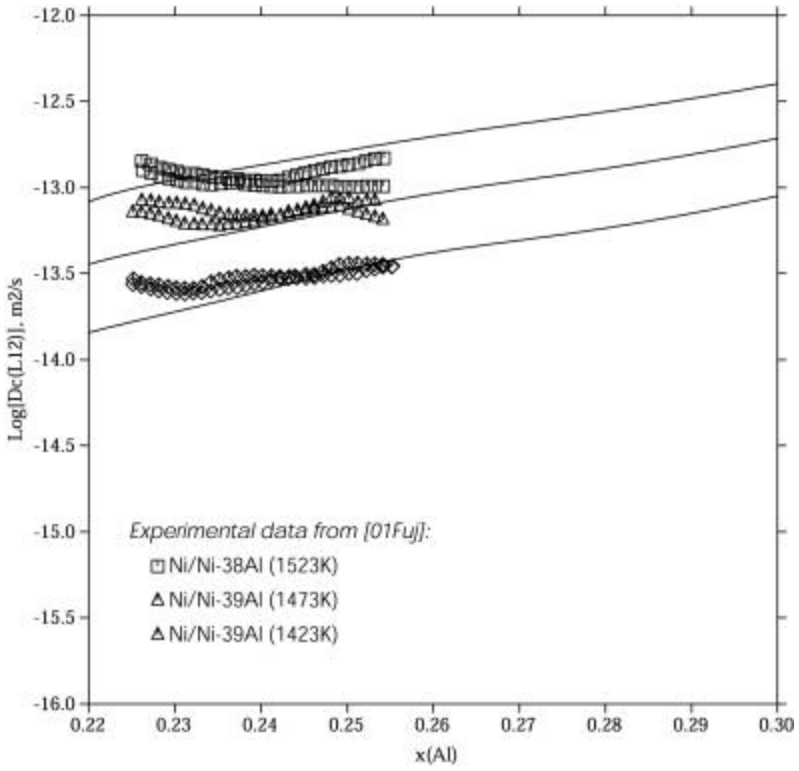
- Energy of reaction can be calculated based on the thermodynamic database.

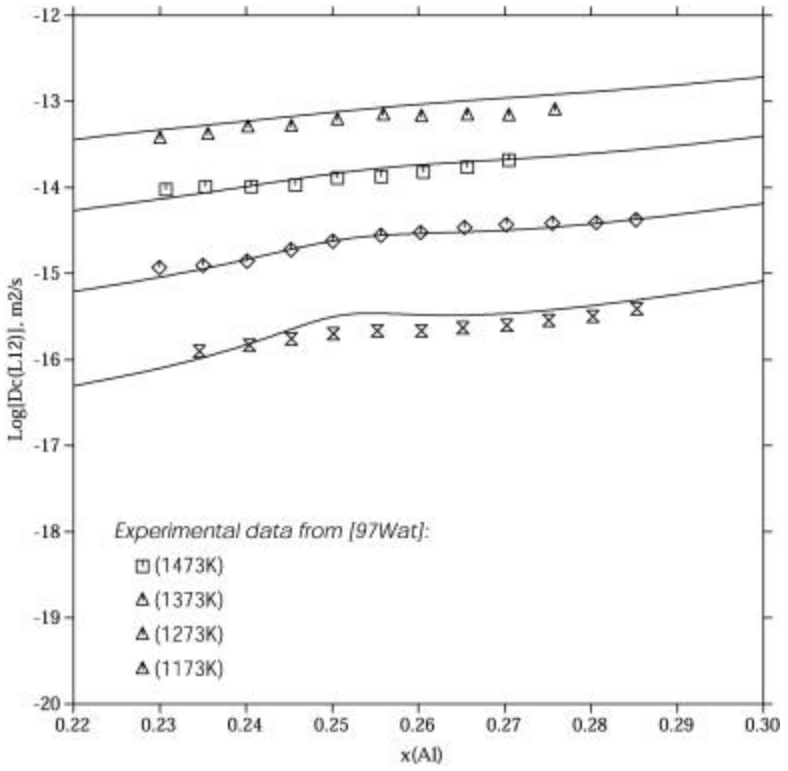
Diffusivity in Stoichiometric Compound (Assessment II)





Diffusivity vs Composition (Assessment II)





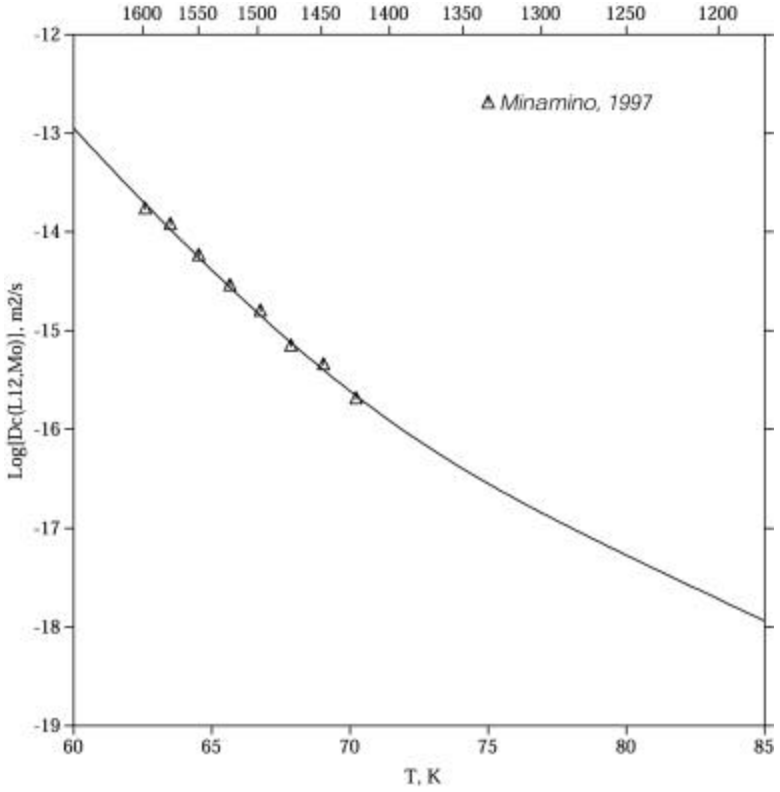
Diffusion in the $L1_2$ Ordered Phase of the Ni-Al-Mo System

Assumptions

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

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

Diffusivity of Mo in Ni_3Al



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.