Self- and Impurity Diffusion in γ-TiAl Single Crystals

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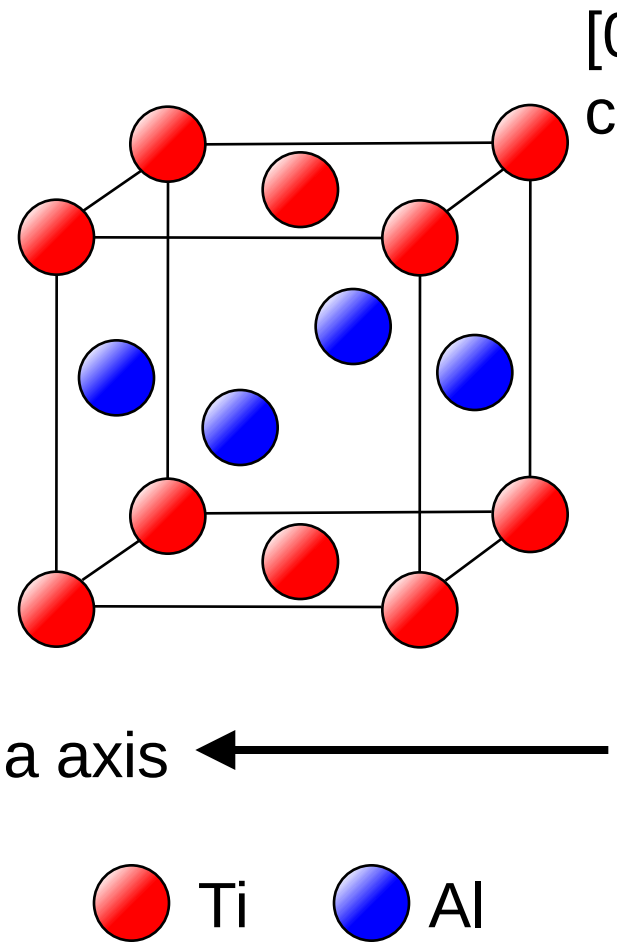
γ-TiAl intermetallic compounds



$L1_0$-type structure

Investigate mechanism of atomic diffusion

Diffusion anisotropy

a-axis direction : D_a

c-axis direction : D_c

using single crystals

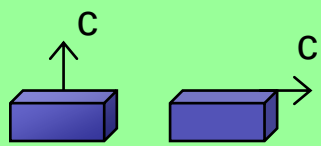
Self- diffusion : Ti, In(Al)

Impurity diffusion: Fe, Ni

Experimental procedure

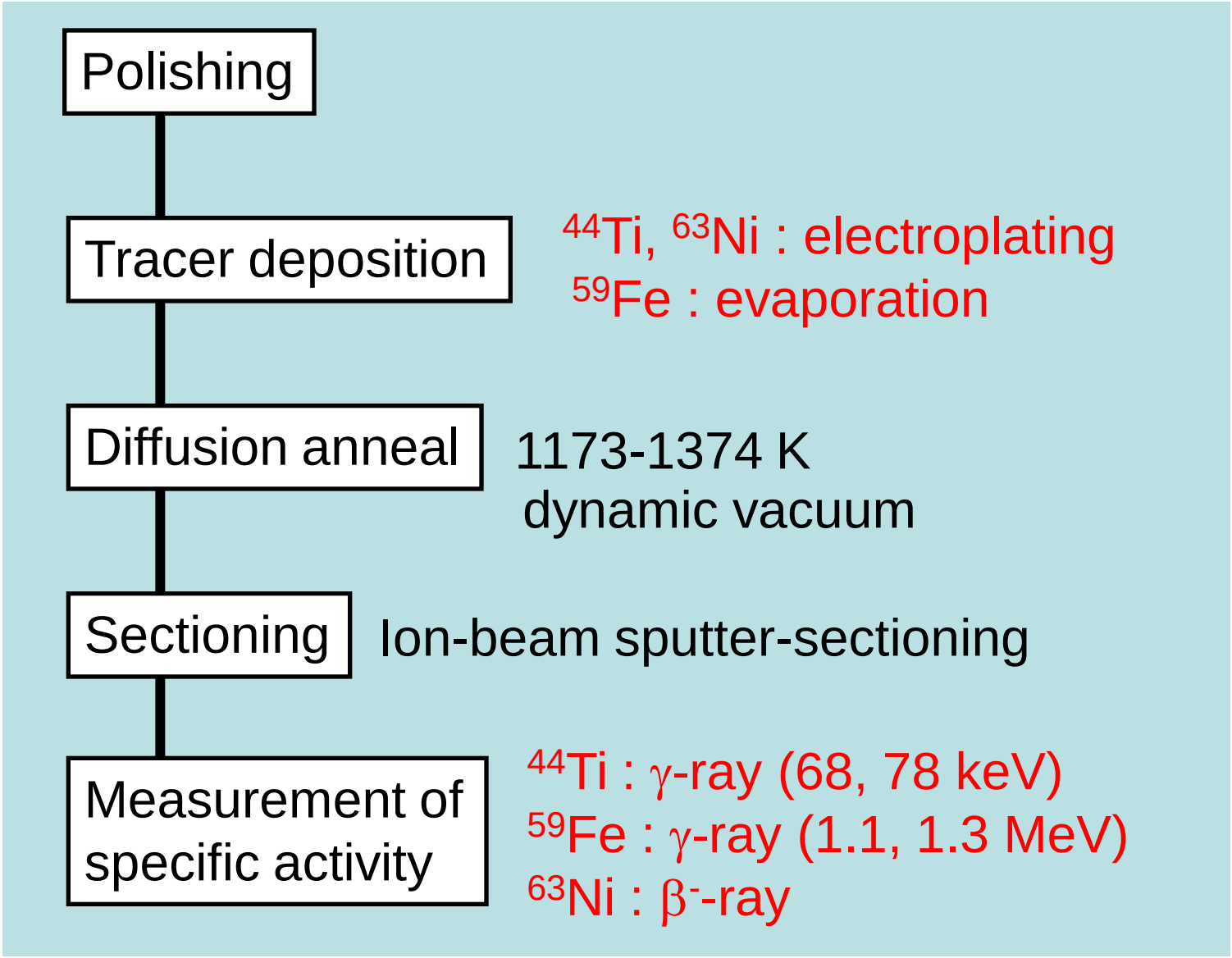
Specimen preparation

- Arc-melting
- Single crystal growth — Floating Zone method
- Anneal for homogeneity — 1353 K, 72 h
- Cutting & polishing — two directions

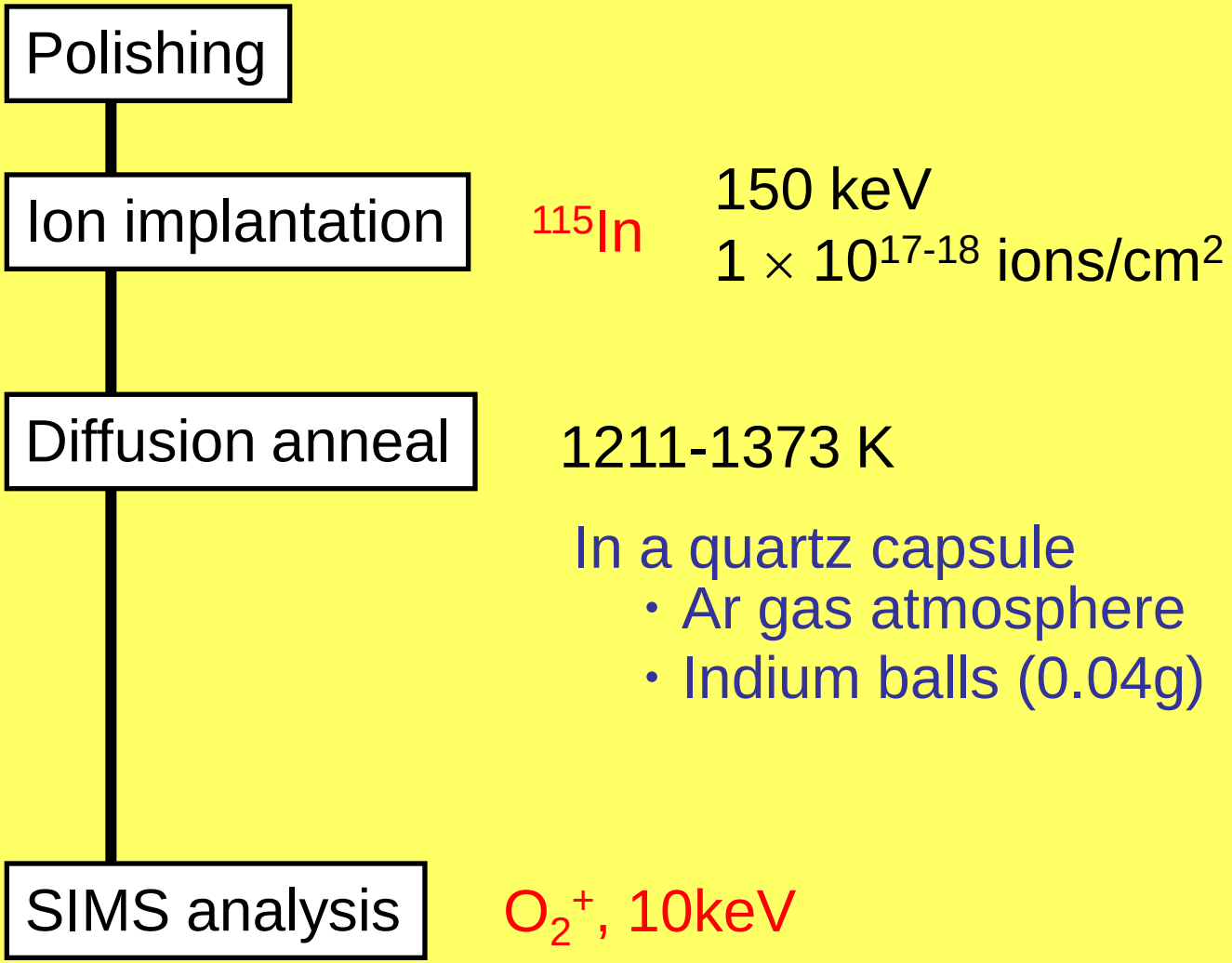


- Composition analysis — 53.2~53.6 mol%Al

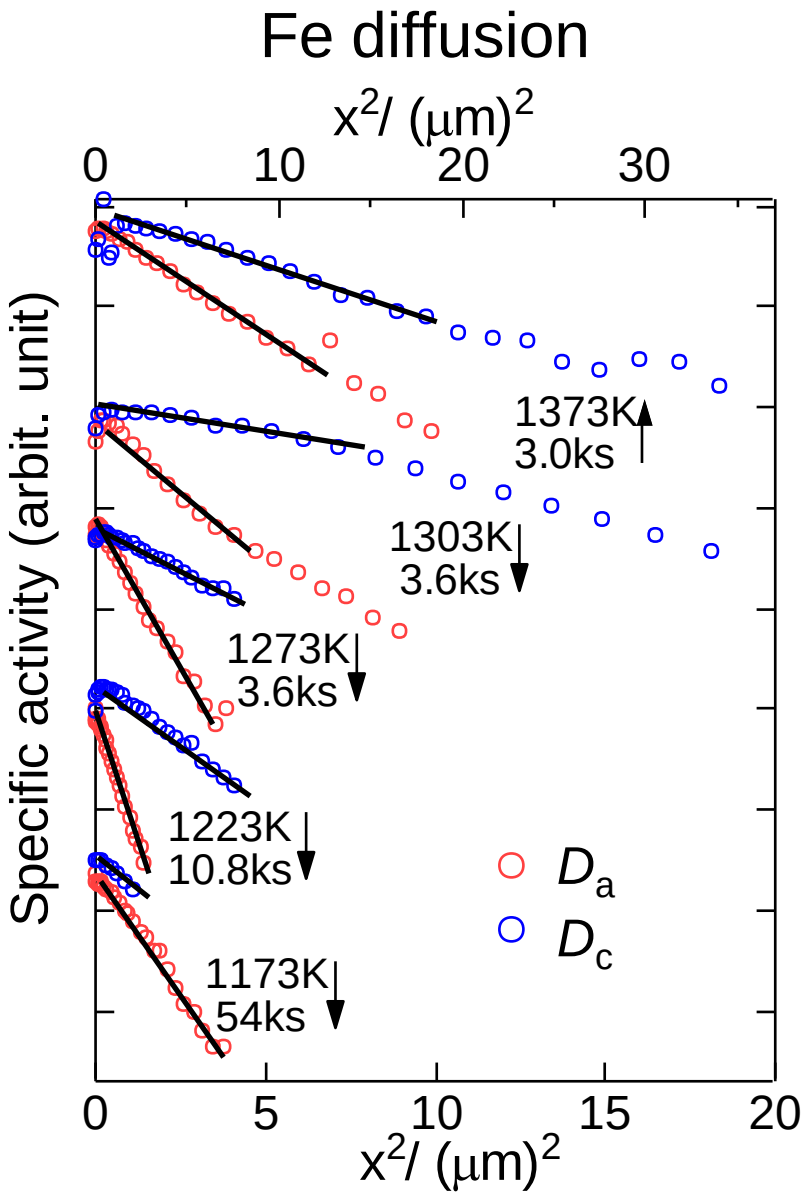
Tracer experiments using radioisotopes *Ti, Fe, Ni in TiAl*

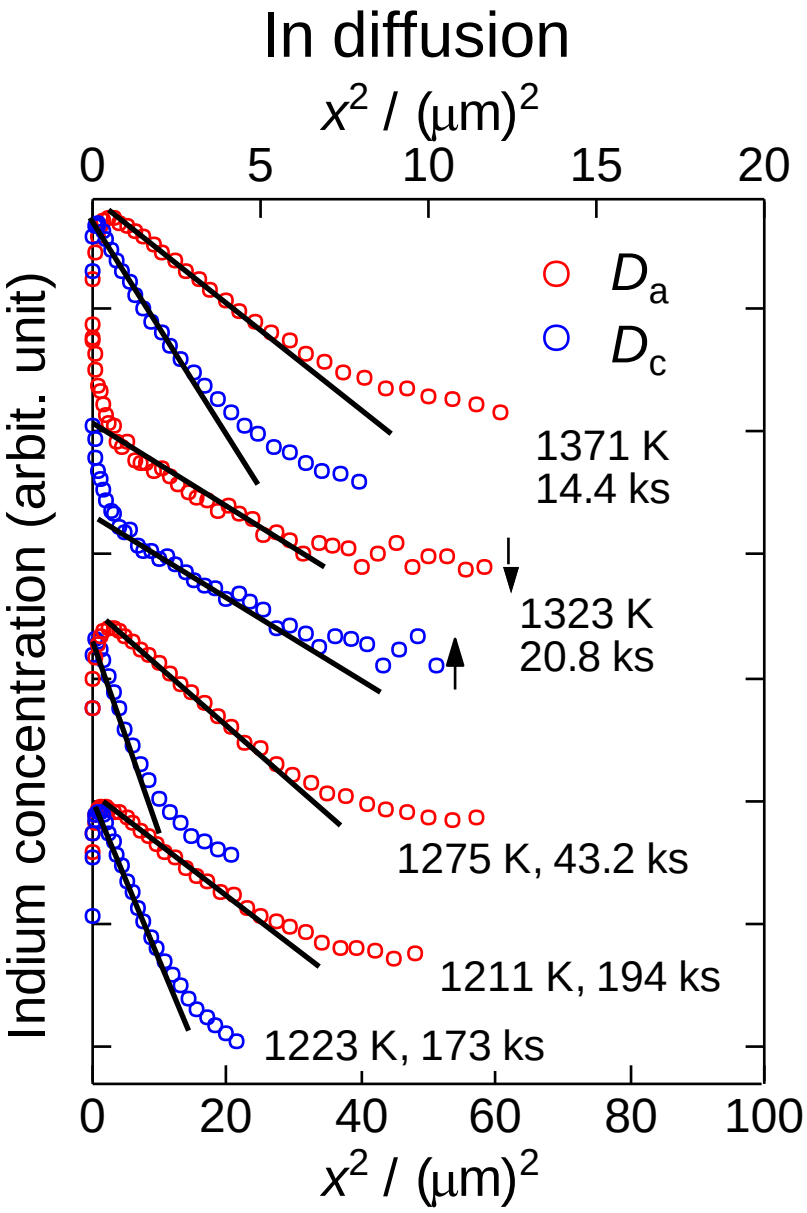


Tracer experiments using SIMS *In in TiAl*

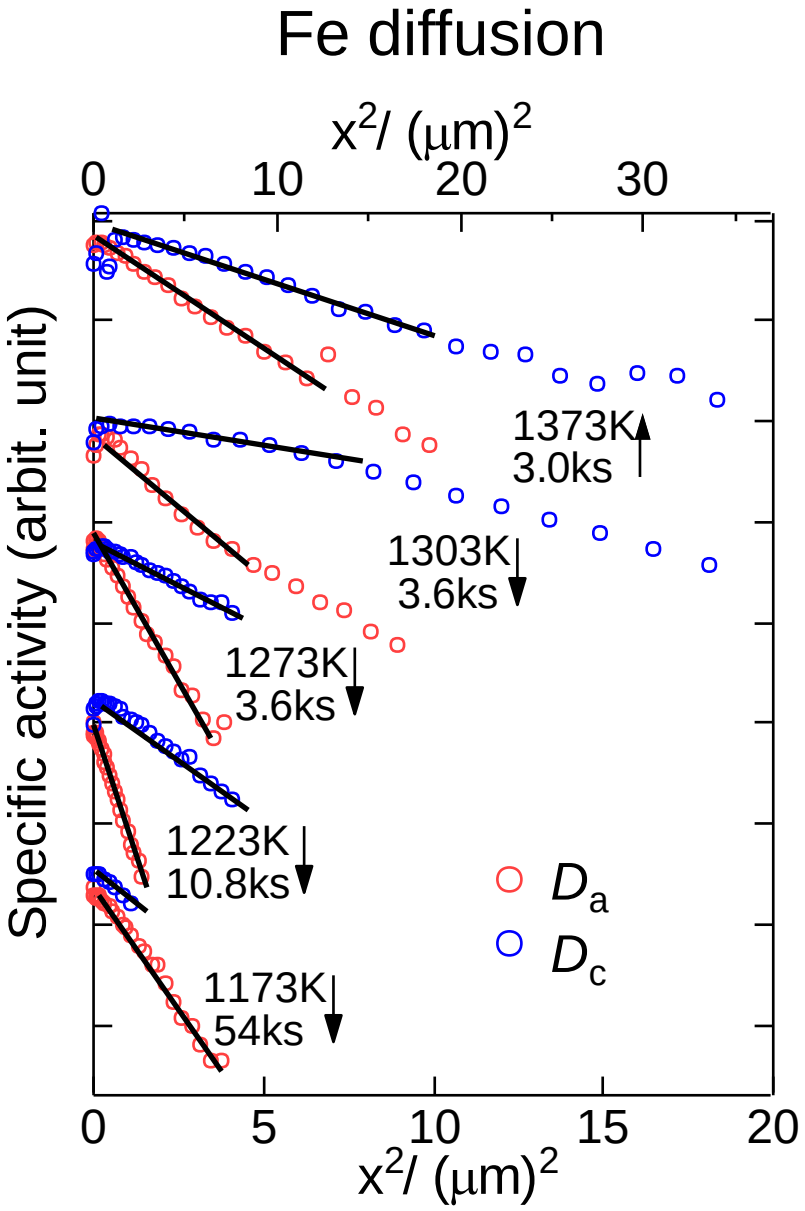


Typical penetration profiles of diffusion in TiAl





Calculation of diffusion coefficient



Thin film solution

$$c = \frac{\alpha}{2\sqrt{\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right)$$

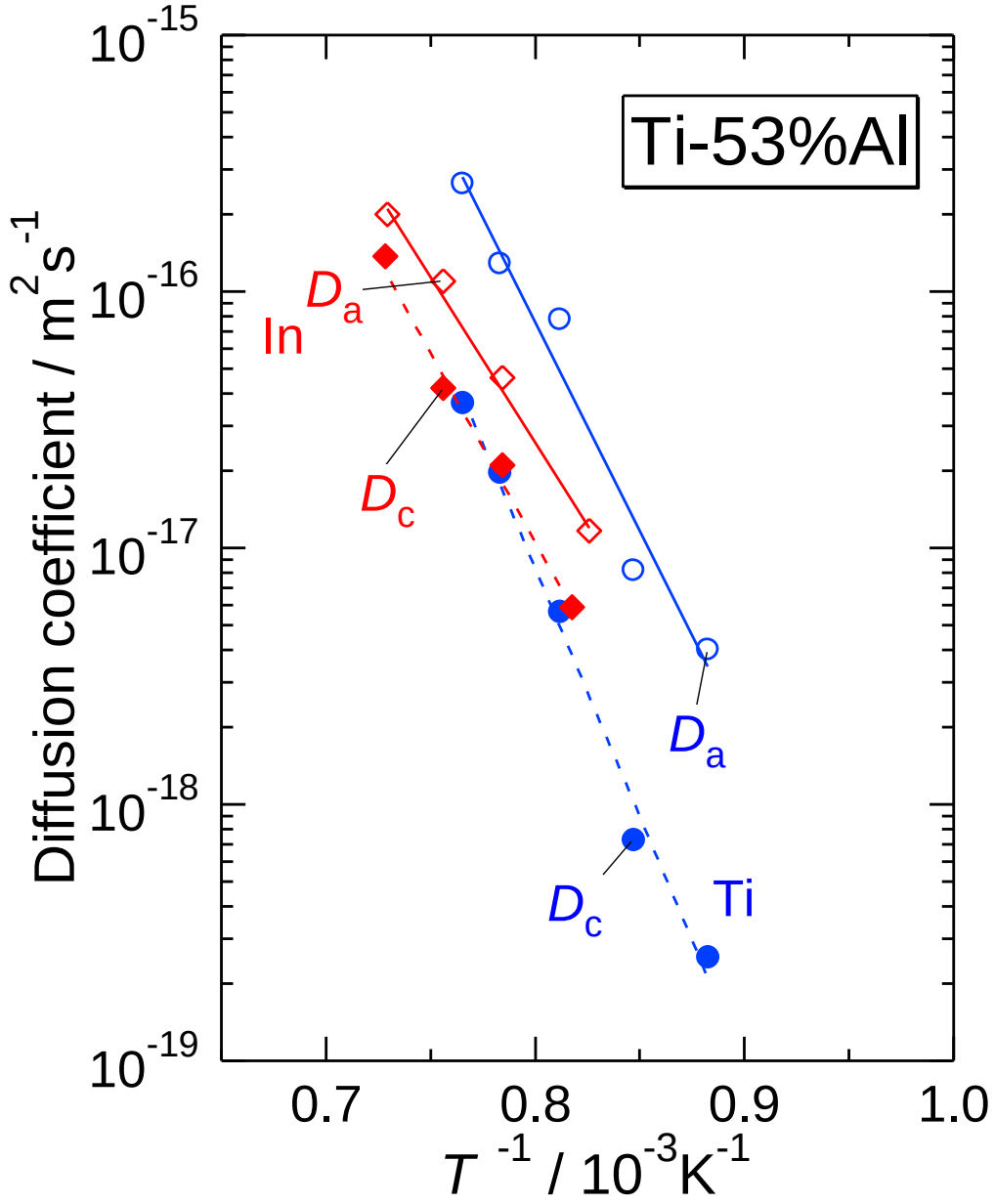
D : diffusion coefficient

x: distance

t : annealing time

$$\ln c = \ln a - \frac{x^2}{4Dt}$$

Diffusion of Ti and In in TiAl single crystal



Anisotropy

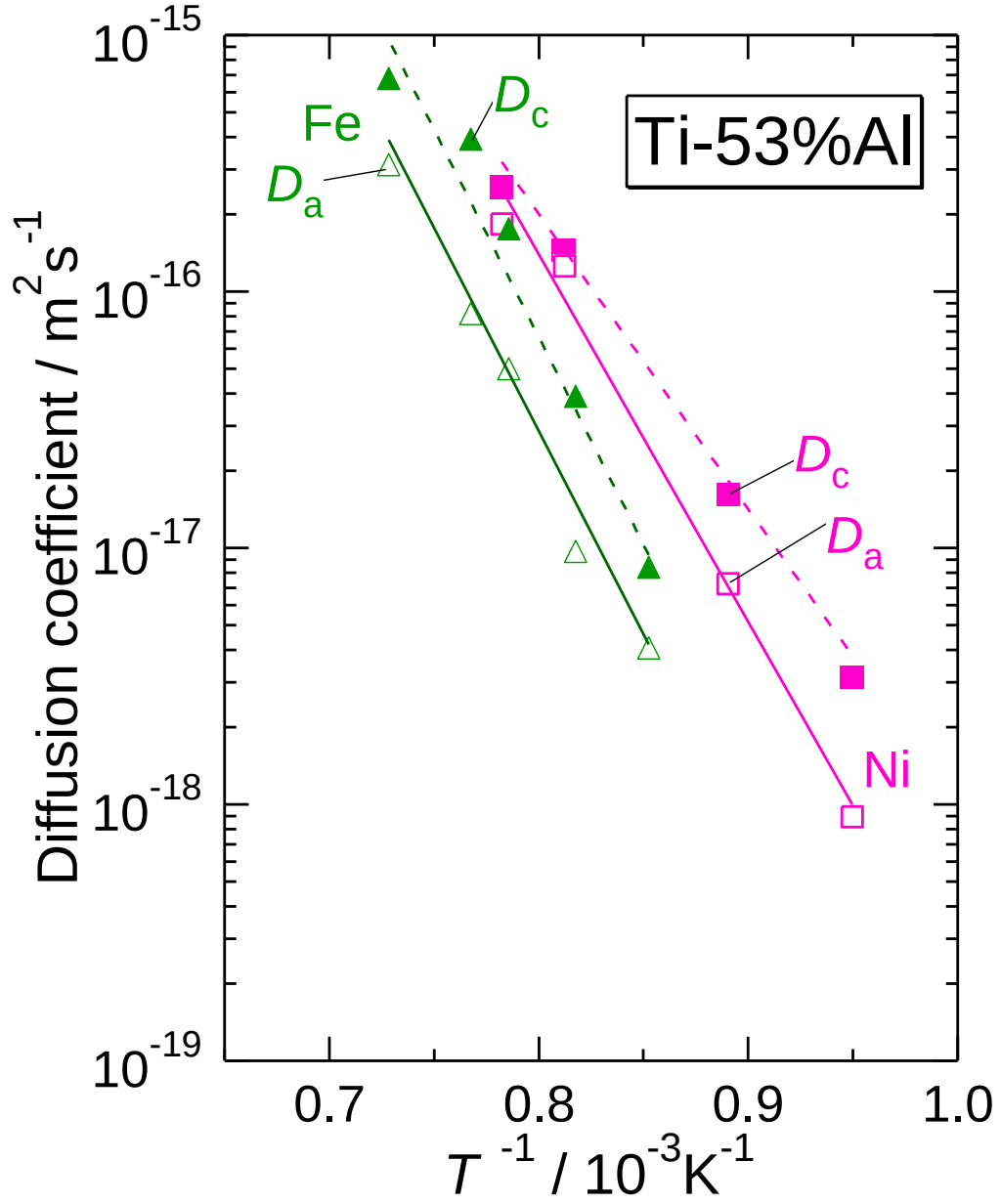
	D_c / D_a
Ti	0.07-0.15
In	0.38-0.69

Activation energy

	Q_c	Q_a
Ti	3.85±0.23	3.22±0.36
In	2.95±0.20	2.57±0.14

eV

Diffusion of Fe and Ni in TiAl single crystal



Anisotropy

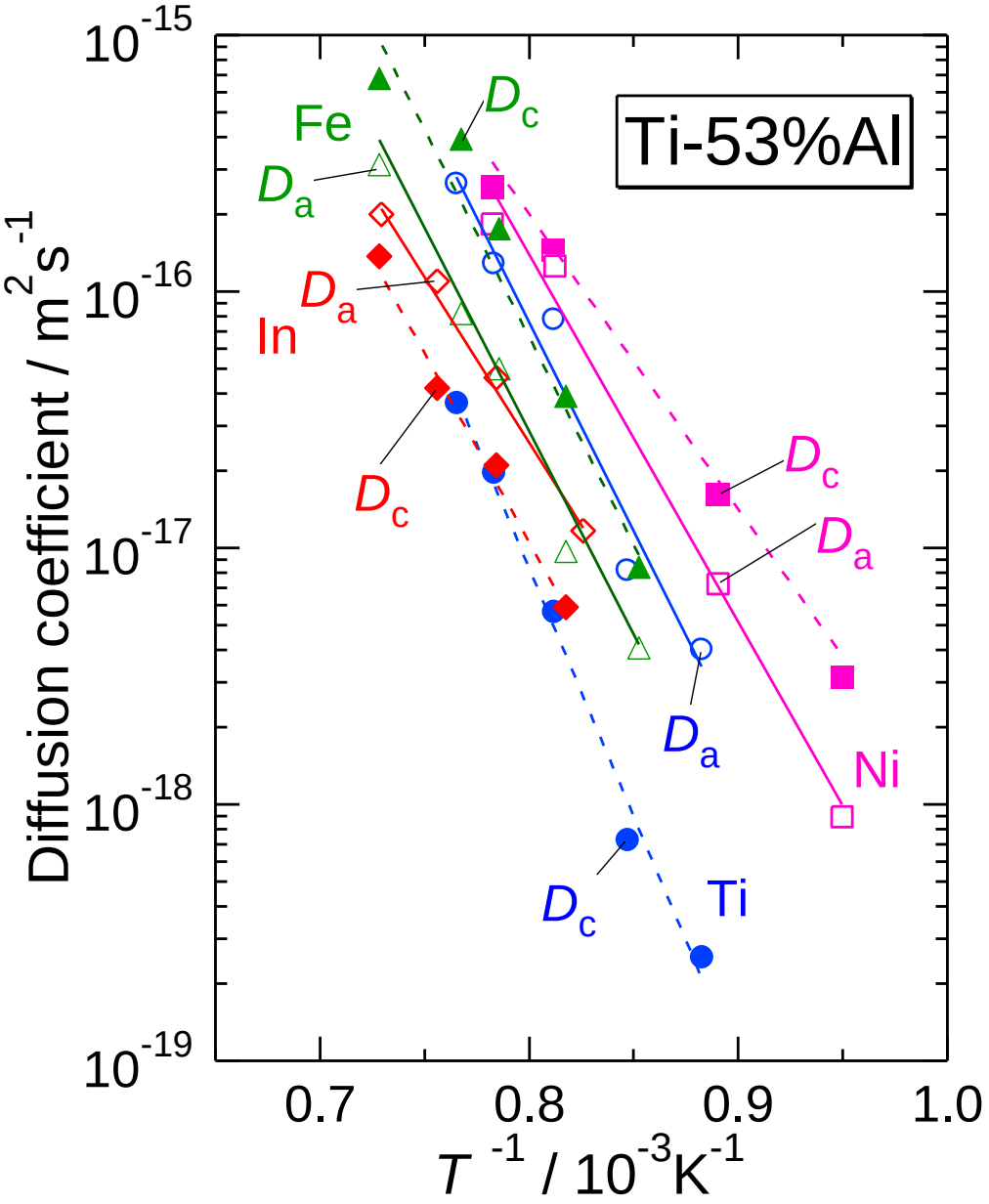
	D_c / D_a
Fe	1.55-4.09
Ni	1.40-3.51

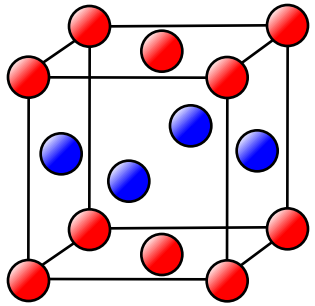
Activation energy

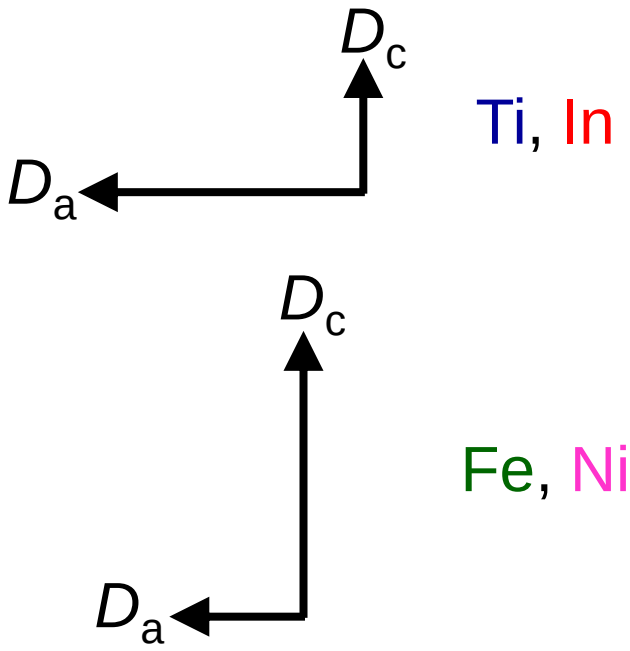
	Q_c	Q_a
Fe	3.21±0.45	3.14±0.31
Ni	2.31±0.07	2.84±0.21

eV

Anisotropy of diffusion in TiAl single crystal

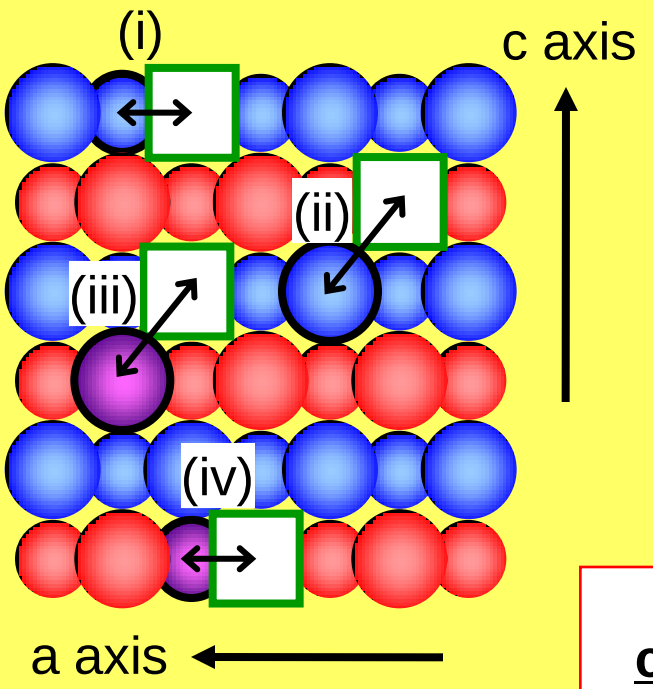






Why ???

Expression of diffusion coefficient for $L1_0$-ordered alloys



Type of jumps of A atoms

(i) Jumps on the planes for A atoms
(ii) Jumps from the A atom planes to B atom planes
(iii) Reverse jumps of (ii)
(iv) Jumps on the plane for B atoms as antisite atoms.

c-axis direction

$$D_c = D_c(\mathrm{ii}, \mathrm{iii})$$

a-axis direction

$$D_a = D_a(\mathrm{i}) + D_a(\mathrm{ii}, \mathrm{iii}) + D_a(\mathrm{iv})$$

Activation energy for Ti diffusion in TiAl single crystal

c-axis direction

$D_c = D_c$(ii+iii)

3.01-3.04

※Calculated for $Ti_{46}Al_{54}$ by Prof. Y. Mishin using embedded atom method. (The unit is eV.)

a-axis direction

$D_a = D_a$(i) + D_a(ii+iii) + D_a(iv)

2.40 3.01-3.04 3.06

Type (i) is predominant

Ti atoms jump on the Ti sublattice!

Calculation

$Q_\perp < Q_{//}$

2.4 3.0

Experiments

$Q_\perp < Q_{//}$

3.2 3.9

Activation energy for Al diffusion in TiAl single crystal

a-axis direction

$D_c = D_c$(ii, iii)

2.60-2.70

c-axis direction

$D_a = D_a$(i) + D_a(ii, iii) + D_a(iv)

2.84 2.60-2.70 2.14

Type (iv) is predominant

Al atoms jump on the Ti sublattice!

Al diffusion (calculation)

$Q_a < Q_c$

2.1 2.7

In diffusion (experiments)

$Q_a < Q_c$

2.6 3.0

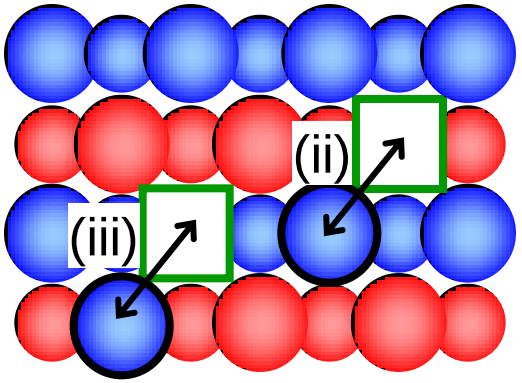
Diffusion mechanism of Fe in TiAl

c-axis direction

$$D_c = D_c(\text{ii, iii})$$

a-axis direction

$$D_a = D_a(\text{i}) + D_a(\text{ii, iii}) + D_a(\text{iv})$$



Assuming that D_a(ii, iii) is predominant,

$$D_c(\text{ii, iii}) = 4\,D_a(\text{ii, iii}) \Rightarrow D_a \leq 4D_c \text{ and } Q_a \approx Q_c$$

Fe diffusion

$D_c / D_a = 2.2\text{-}4.8$

$Q_c \approx Q_a$

⇒ Fe atoms diffuse on both Ti and Al sublattices !

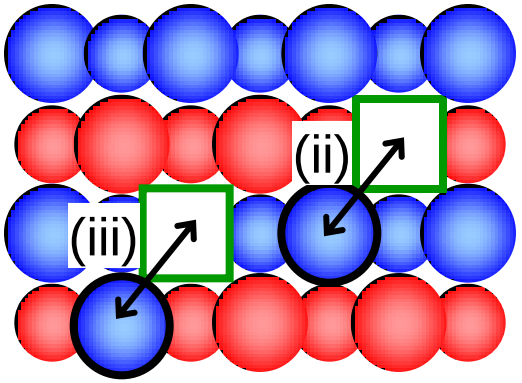
Diffusion mechanism of Ni in TiAl

c-axis direction

$$D_c = D_c(\text{ii, iii})$$

a-axis direction

$$D_a = D_a(\text{i}) + D_a(\text{ii, iii}) + D_a(\text{iv})$$



Assuming that D_a(ii, iii) is predominant, ➡ $D_a < 4D_c$ and $Q_a \approx Q_c$

Ni diffusion

$D_c / D_a = 1.4\text{-}3.6$

$Q_c < Q_a$

➡

Type (ii, iii) may be not predominant !

⬇

Mixed mechanism??

Conclusions

Ti and In in TiAl

Ti: $D_c / D_a = 0.07\text{-}0.15$ $Q_c > Q_a$

In: $D_c / D_a = 0.38\text{-}0.69$ $Q_c > Q_a$

Ti atoms jump on Ti sublattice.

In atoms jump on Ti sublattice.

Fe and Ni in TiAl

Fe and Ni : opposite anisotropy to Ti and In

Fe : $D_c / D_a = 1.55\text{-}4.09$ $Q_c \approx Q_a$

Ni: $D_c / D_a = 1.40\text{-}3.51$ $Q_c < Q_a$

Fe atoms jump on both Ti and Al sublattice.

For Ni diffusion, further investigation is necessary.

Concluding remark

One can infer diffusion mechanisms in $L1_0$-ordered alloys by investigating diffusion anisotropy

For diffusion perpendicular to the [001] axis,

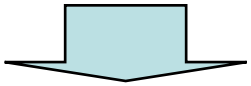
$$D_a = D_a(\text{i}) + D_a(\text{ii, iii}) + D_a(\text{iv})$$

(a) the process (i) or (iv) is predominant

$\rightarrow Q_c > Q_a$, $D_c > D_a$ (the case of Ti or Al)

(b) the process (ii, iii) is predominant

$\rightarrow Q_c \approx Q_a$, $D_c < D_a$ (the case of Fe)



$Q_c > Q_a$, $D_c > D_a \rightarrow$ the process (i) or (iv) is predominant.

$Q_c \approx Q_a$, $D_c < D_a \rightarrow$ the process (ii, iii) is predominant.