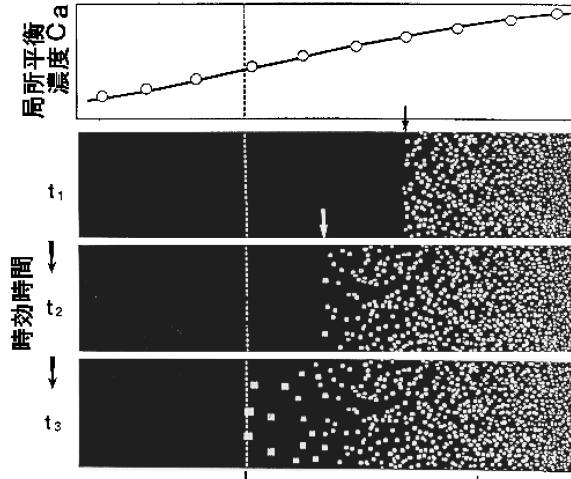


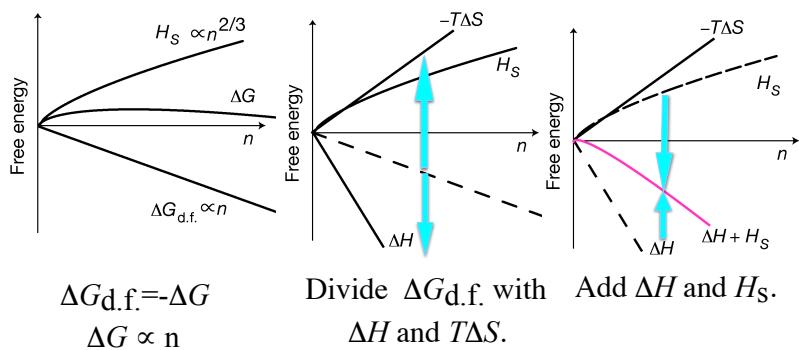
- Fe-Cu系の核生成
 - 核生成の自由エネルギー, 添加元素, 空孔
 - キネティックMC (速度論との接続), 热振動

Ni-Al組成傾斜合金からのNi₃Alの析出

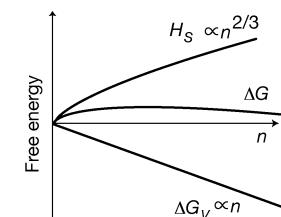


宮崎亨, まりあ, vol.48 (2009), 397-403, 図12.

New grouping of energies

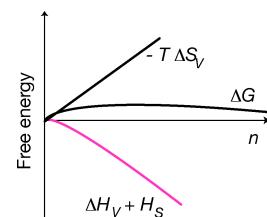


Classical treatment



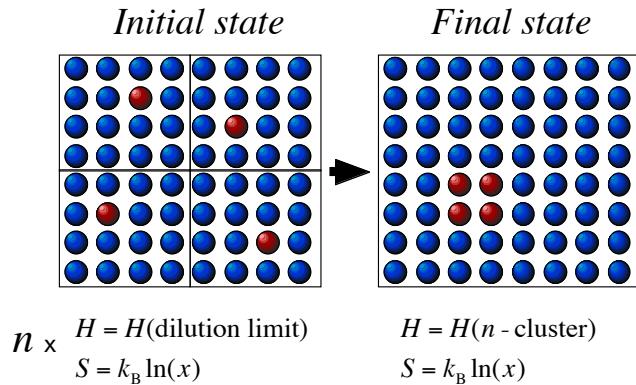
$$\begin{aligned}\Delta G(n) &= \Delta G_v + H_s \\ &= \Delta H_v - T \Delta S_v + H_s \\ &= \boxed{\Delta H_v + H_s} - T \Delta S_v\end{aligned}$$

New treatment

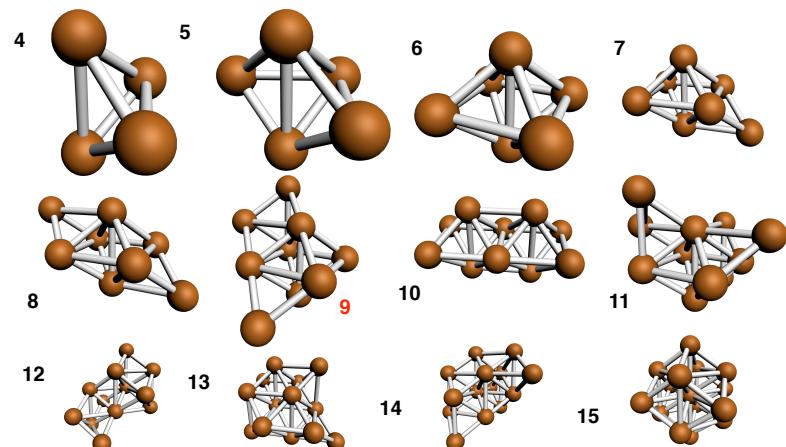


$$\begin{aligned}\Delta S_v &\sim k_B(n-1) \ln(x) \\ T. Kamijo and H. Fukutomi, Phil. Mag. A, 48(1983), 685.\end{aligned}$$

Illustration of precipitation

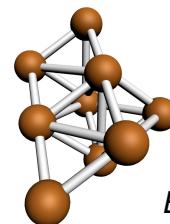


Cluster configurations



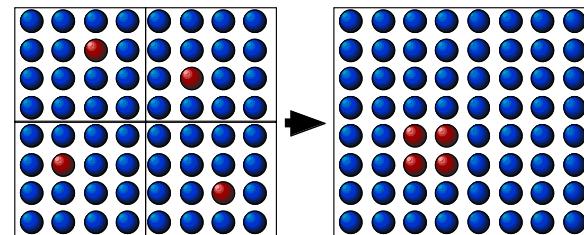
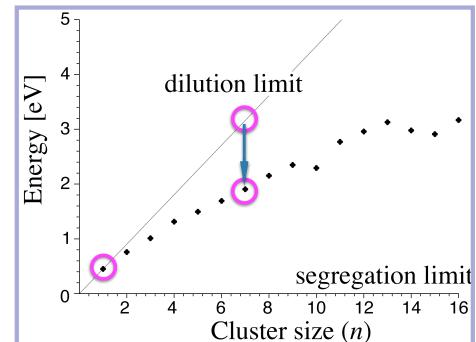
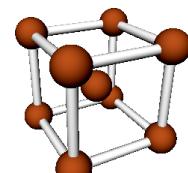
Cluster energy ($n = 9$)

$$E_{\text{cluster}} = 2.35 \text{ eV}$$

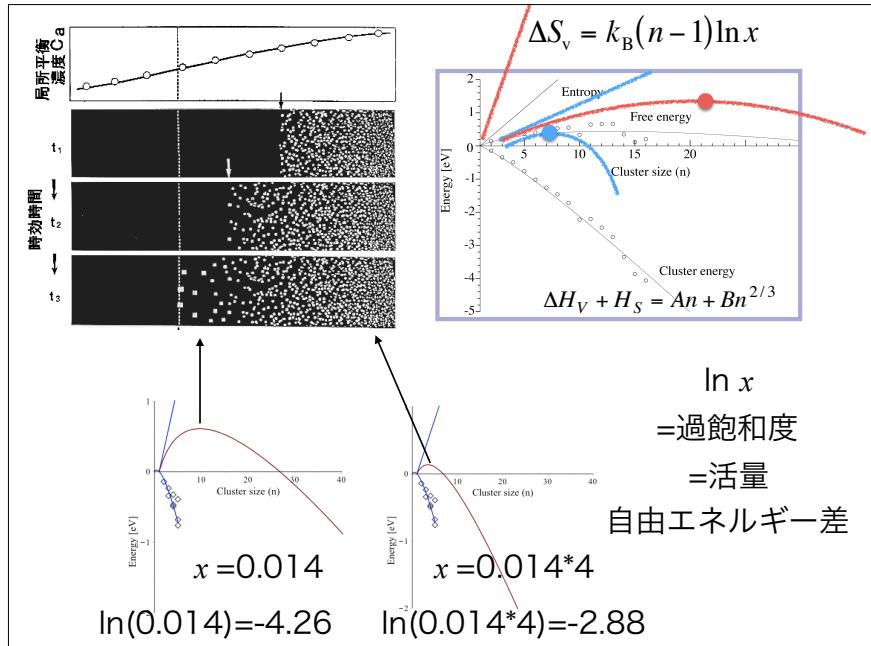
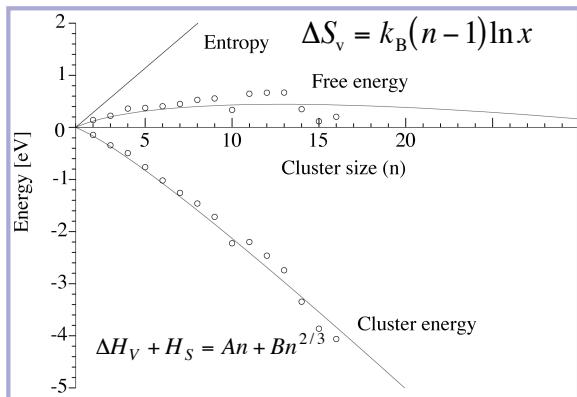


$$\begin{aligned} E_{\{011\}} &= 0.24 \text{ J/m}^2 \\ E_{\{111\}} &= 0.38 \text{ J/m}^2 \\ E_{\{001\}} &= 0.60 \text{ J/m}^2 \end{aligned}$$

$$E_{\text{cluster}} = 2.97 \text{ eV}$$

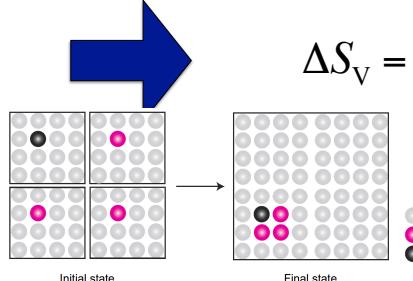


Cluster free energy



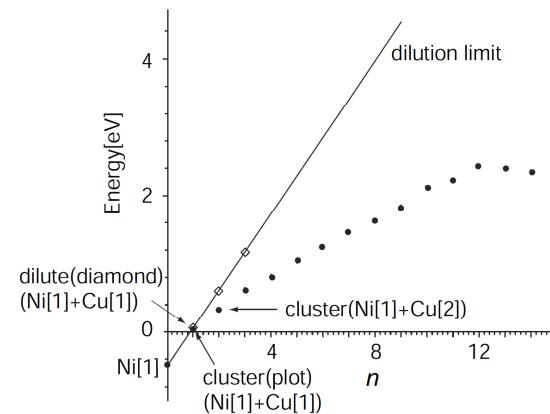
Ternary Entropy expression

$$\Delta S_v = k_B(n-1)\ln(x_{Cu})$$

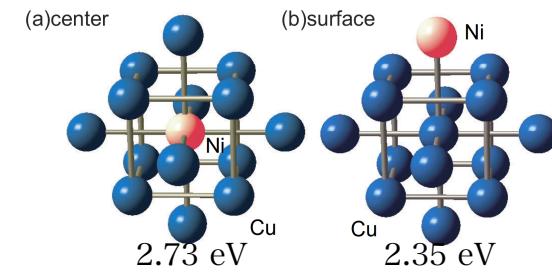
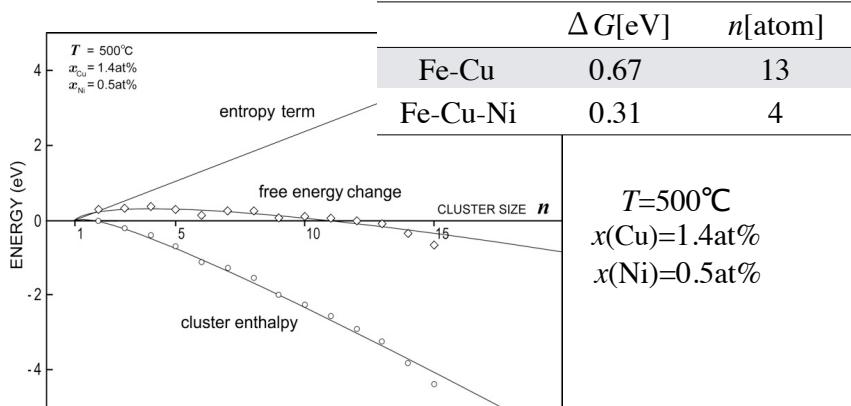


$$\Delta S_v = k_B \left\{ \begin{aligned} & (n-1)\ln(x_{Cu}) \\ & + \ln \frac{x_{Ni}}{x_{Cu}}(n-1) \\ & + \ln n \end{aligned} \right\}$$

Cluster enthalpy



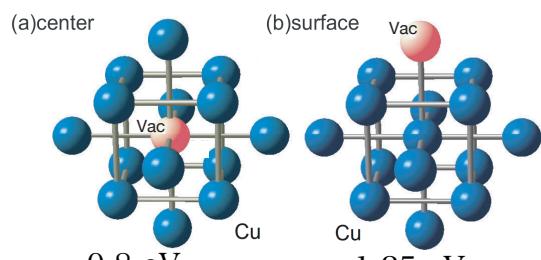
Free energy for Fe-Cu-Ni



Interaction parameter

Fe-Cu	59.0meV
Cu-Ni	-0.7meV
Fe-Ni	0.5meV

Vacancy + Cu cluster



$$\text{Evac}(\text{Cu}) = 0.6 \text{ eV}$$

$$\text{Evac}(\text{Fe}) = 2.3 \text{ eV}$$