Appendices of "Coherent phase equilibria of systems with large lattice mismatch"

Anh Thu Phan, Aïmen E. Gheribi, Patrice Chartrand

Appendix A: Formulation of the elastic Gibbs energy

A.1 Small deformation regime

a. *The [100] habit plane*

According to the assumption stated by Cahn,[1-4] two elastic strains related to the difference of the lattice parameter (a') of the solid solution with the fluctuated composition (x) and that (a_0) with the overall composition (x_0) are $\varepsilon_2 = \varepsilon_3 = \varepsilon = \frac{a'-a_0}{a_0}$, and the corresponding stresses are $\sigma_2 = \sigma_3 = \sigma$:

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon \\ \varepsilon \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{22} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{12} & S_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{44} \end{bmatrix} \cdot \begin{bmatrix} 0 \\ \sigma \\ \sigma \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{A.1}$$

where S_{ij} are the elastic compliance of the cubic material and where i and j are Voigt notations. Solving equation (A.1), we obtain:

$$\sigma = \frac{\varepsilon}{(S_{11} + S_{12})} = \frac{\varepsilon_1}{2S_{12}} \tag{A.2}$$

The elastic energy stored in the crystal in the small deformation regime is estimated as follows:

$$f_{el}^{s} = \frac{1}{2}\sum S_{ij}\sigma_i\sigma_j \tag{A.3}$$

Substituting equation (A.2) into equation (A.3), the elastic energy stored becomes:

$$f_{el}^{s} = Y_{100}^{s} \cdot \varepsilon^2 \tag{A.4}$$

with:

$$Y_{100}^{s} = \frac{1}{(S_{11} + S_{12})} = \frac{(C_{11} - C_{12}) \cdot (C_{11} + 2C_{12})}{C_{11}} \tag{A.5}$$

where C_{ij} are the elastic constants of the cubic material. Note that the expression of Y_{100}^{s} in equation (A.5) is exactly what was reported by Cahn.[1-4]

b. *The [111] habit plane*

In order to reproduce the elastic Gibbs energy of [111] plane reported by Cahn,[1-4] we will consider a general stress-strain relation in an isotropic material:

$$\begin{bmatrix}\varepsilon\\ \varepsilon_2\\ \varepsilon_3\\ \varepsilon_4\\ \varepsilon_5\\ \varepsilon_6\end{bmatrix}=\begin{bmatrix}S_{11} & S_{12} & S_{12} & 0 & 0 & 0\\ S_{12} & S_{22} & S_{12} & 0 & 0 & 0\\ S_{12} & S_{12} & S_{33} & 0 & 0 & 0\\ 0 & 0 & 0 & S_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & S_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & S_{44}\end{bmatrix}\cdot\begin{bmatrix}\sigma_1\\ k_2\sigma_1\\ k_3\sigma_1\\ \sigma_4\\ k_5\sigma_4\\ k_6\sigma_4\end{bmatrix} \tag{A.6}$$

where k_2, k_3, k_4, k_5 are real numbers.

So, the elastic energy stored in the crystal within the small deformation regime is estimated as follow:

$$f_{el}^{s}=\frac{1}{2}\sum S_{ij}\sigma_i\sigma_j=\frac{1}{2}\{S_{11}{\sigma_1}^2(1+{k_2}^2+{k_3}^2)+2S_{12}{\sigma_1}^2(k_2+k_3+k_2k_3)+S_{44}{\sigma_4}^2(1+{k_5}^2+{k_6}^2)\} \tag{A.7}$$

Substitute $\sigma_1=\frac{\varepsilon}{(S_{11}+k_2S_{12}+k_3S_{12})}$ derived from equation (A.6) and $\sigma_4=m\sigma_1$ (where m is a real number) into equation (A.7), we obtain:

$$f_{el}^{s}=\frac{1}{2}\frac{\varepsilon^2}{(S_{11}+k_2S_{12}+k_3S_{12})^2}\{S_{11}(1+{k_2}^2+{k_3}^2)+2S_{12}(k_2+k_3+k_2k_3)+m^2S_{44}(1+{k_5}^2+{k_6}^2)\}=Y_{111}^{s}\cdot\varepsilon^2 \tag{A.8}$$

i.e.,

$$Y_{111}^{s}=\frac{\{S_{11}(1+{k_2}^2+{k_3}^2)+2S_{12}(k_2+k_3+k_2k_3)+m^2S_{44}(1+{k_5}^2+{k_6}^2)\}}{2(S_{11}+k_2S_{12}+k_3S_{12})^2} \tag{A.9}$$

If the expression of Y_{111}^{s} in equation (A.9) is equivalent to Y_{111}^{s} obtained from Cahn's approach[1-4], we should have:

$$\frac{\{S_{11}(1+{k_2}^2+{k_3}^2)+2S_{12}(k_2+k_3+k_2k_3)+m^2S_{44}(1+{k_5}^2+{k_6}^2)\}}{2(S_{11}+k_2S_{12}+k_3S_{12})^2}=\frac{6}{4(S_{11}+2S_{12})+S_{44}} \tag{A.10}$$

If there exists an exact stress-strain relation for the calculation of the elastic energy corresponding to the [111] habit plane, there exist values of k_2, k_3, k_5, k_6 satisfying equation (A.10) for every S_{11}, S_{12}, and S_{44}. However, since no set of k_2, k_3, k_5, and k_6 satisfying equation (A.10) is found, it is impossible to find a suitable stress-strain relation which could reproduce the elastic Gibbs energy of Cahn's approach for the [111] habit plane.[1-4] In order to estimate the elastic Gibbs energy stored in the [111] habit plane, in this study, we propose another stress-strain relation for calculating the coherent miscibility gap as follows:

$$\begin{bmatrix}\varepsilon\\ \varepsilon_2\\ \varepsilon_2\\ \varepsilon\\ 0\\ 0\end{bmatrix}=\begin{bmatrix}S_{11} & S_{12} & S_{12} & 0 & 0 & 0\\ S_{12} & S_{11} & S_{12} & 0 & 0 & 0\\ S_{12} & S_{12} & S_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & S_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & S_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & S_{44}\end{bmatrix}\cdot\begin{bmatrix}\sigma_1\\ 0\\ 0\\ \sigma_4\\ 0\\ 0\end{bmatrix} \tag{A.11}$$

This stress-strain relation is proposed to reproduce the experimental data of the [111] coherent miscibility gap in our case studies (shown in part 3). Like the [100] habit plane, the elastic energy stored in the crystal for small deformation is estimated as follows:

$$f_{el}^{s}=Y_{111}^{s}\cdot\varepsilon^2 \tag{A.12}$$

with:

$$Y_{111}^{s}=\frac{1}{2}\left[\frac{1}{S_{11}}+\frac{1}{S_{44}}\right]=\frac{1}{2}\left[\frac{(C_{11}-C_{12})\cdot(C_{11}+2C_{12})}{C_{11}+C_{12}}+C_{44}\right] \tag{A.13}$$

After obtaining the formulae of Y depending on the elastic constants C_{ij} corresponding to the [100] or [111] habit plane, in a similar way to Cahn's approach,[1-4] we consider a sinusoïdal plane wave fluctuation of the composition, then the elastic strain can be written as:

$$\varepsilon = \eta(x - x_0) = \eta A cos(\boldsymbol{\beta} \cdot \boldsymbol{r}) \qquad \text{(A.14)}$$

where x_0 is the overall composition and x is the local composition of the solid solution and the composition fluctuates as $x - x_0 = A cos(\boldsymbol{\beta} \cdot \boldsymbol{r})$; $\eta = \frac{1}{a}\frac{\partial a}{\partial x}$ is the rate of change of the lattice constants with composition. If $\frac{\partial a}{\partial x}$ is a constant, it is called Vegard's coefficient. According to Cahn,[1-4] the total free energy of volume V of an isotropic solid solution free from imperfections in which the molar volume is independent of both composition and pressure is:

$$F = \int_V \{f'(x) + Y^s \eta^2 (x - x_0)^2 + \kappa(\nabla x)^2\}\, dV \qquad \text{(A.15)}$$

where $f'(x)$ is the Helmholtz free energy of a unit volume of homogeneous materials of composition x and $\kappa(\nabla x)^2$ is the first term of an expansion representing the increase in free energy due to the introduction of a gradient of composition. Expanding $f'(x)$ in a Taylor's series with $x - x_0 = A cos(\boldsymbol{\beta} \cdot \boldsymbol{r})$ and integrating the above equation, we obtain the change in free energy per unit volume between the initial homogeneous solution of concentration x_0 and the inhomogeneous solution of concentration x:

$$\frac{\Delta F}{V} = \frac{1}{4} A^2 \left\{ \frac{\partial^2 f'}{\partial x^2} + 2Y^s \eta^2 + 2\kappa \beta^2 \right\} \qquad \text{(A.16)}$$

If the free energy change $\frac{\Delta F}{V}$ is negative for some wave vectors $\boldsymbol{\beta}$, then the solution is unstable to infinitesimal fluctuations with those wave vectors. Otherwise, the solution is stable to all infinitesimal fluctuations. The spinodal curve for a particular direction of the wave vector is given by the condition that the solution just be unstable to fluctuations of infinite wavelength but stable to fluctuations of finite wavelength in that directions, that is, the spinodal is given by:

$$\frac{\partial^2 f'}{\partial x^2} + 2Y^s \eta^2 = 0 \qquad \text{(A.17)}$$

Equation (A.17) is applied for a volume unit of the solid solution. Hence, for a molar volume of an isotropic material under coherent spinodal decomposition:

$$\frac{\partial^2 F}{\partial x^2} + 2V_m Y^s \eta^2 = 0 \qquad \text{(A.18)}$$

where F is the molar Helmholtz free energy. In fact, the molar Gibbs energy $G = F - PV$. Since the second derivative of PV versus x is neglected, equation (A.18) becomes:

$$\frac{\partial^2 G}{\partial x^2} + 2V_m Y^s \eta^2 = 0 \qquad \text{(A.19)}$$

A.2 Large deformation regime

a. *The [100] habit plane*

Corresponding to the stress-strain relation developed for calculating the elastic Gibbs energy of [100] coherence in the small deformation regime in equation (A.1), the Cauchy stress tensor is $\begin{bmatrix} 0 & 0 & 0 \\ 0 & \sigma & 0 \\ 0 & 0 & \sigma \end{bmatrix}$ and the strain tensor is $\begin{bmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{bmatrix}$. The elastic energy stored in the crystal is estimated from the Almansi strain and the second Poila-Kirchhoff stress. The matrix deformation matrix is:

$$[\boldsymbol{F}] = \begin{bmatrix} \varepsilon_1 + 1 & 0 & 0 \\ 0 & \varepsilon + 1 & 0 \\ 0 & 0 & \varepsilon + 1 \end{bmatrix} = \begin{bmatrix} k\varepsilon + 1 & 0 & 0 \\ 0 & \varepsilon + 1 & 0 \\ 0 & 0 & \varepsilon + 1 \end{bmatrix} \tag{A.19}$$

Where $\varepsilon_1 = k\varepsilon$ with $k = \frac{2S_{12}}{(S_{11}+S_{12})}$ is a real number. Hence,

$$\boldsymbol{J} = |\det \boldsymbol{F}| = (k\varepsilon + 1) \cdot (\varepsilon + 1)^2 \tag{A.20}$$

The right Cauchy-Green deformation tensor

$$[\boldsymbol{C}] = [\boldsymbol{F}]^{\boldsymbol{T}} \cdot [\boldsymbol{F}] = \begin{bmatrix} (k\varepsilon + 1)^2 & 0 & 0 \\ 0 & (\varepsilon + 1)^2 & 0 \\ 0 & 0 & (\varepsilon + 1)^2 \end{bmatrix} \tag{A.21}$$

The Almansi-Lagrange strain tensor:

$$[\boldsymbol{e}] = \frac{1}{2}\left([\boldsymbol{I}] - [\boldsymbol{C}^{-1}]\right) = \frac{1}{2}\begin{bmatrix} 1 - \frac{1}{(k\varepsilon + 1)^2} & 0 & 0 \\ 0 & 1 - \frac{1}{(\varepsilon + 1)^2} & 0 \\ 0 & 0 & 1 - \frac{1}{(\varepsilon + 1)^2} \end{bmatrix} \tag{A.22}$$

The second Piola-Kirchhoff stress tensor:

$$[\widetilde{\boldsymbol{T}}] = [\boldsymbol{F}^{-1}] \cdot \boldsymbol{J} \cdot [\boldsymbol{T}] \cdot [\boldsymbol{F}^{-1}]^{\boldsymbol{T}} = (k\varepsilon + 1) \cdot \sigma \cdot \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{A.23}$$

Similarly, the elastic energy stored in the crystal is estimated as follow:

$$f_{el}^{l} = \frac{1}{2}\sum e_{ij} \cdot \tilde{T}_{ij} = \frac{1}{2} \cdot (k\varepsilon + 1)\sigma\left[1 - \frac{1}{(\varepsilon + 1)^2}\right] \tag{A.24}$$

Substituting equation (A.2) into equation (A.24), we obtain the expression for the stored elastic energy in the crystal in large deformation regime:

$$f_{el}^{l} = Y_{100}^{l} \cdot \varepsilon^2 \tag{A.25}$$

with:

$$Y_{100}^{l} = \frac{1}{(S_{11} + S_{12})} \cdot \left[\frac{S_{12}}{(S_{11} + S_{12})} + \frac{S_{11}}{(S_{11} + S_{12})(\varepsilon + 1)^2} + \frac{\varepsilon}{2(\varepsilon + 1)^2}\right] \tag{A.26}$$

b. *The [111] habit plane*

Similarly, using the Cauchy stress tensor $[\boldsymbol{T}] = \begin{bmatrix} \sigma & 0 & 0 \\ 0 & 0 & k\sigma \\ 0 & k\sigma & 0 \end{bmatrix}$ and strain tensor $\begin{bmatrix} \varepsilon & 0 & 0 \\ 0 & \varepsilon_2 & \varepsilon/2 \\ 0 & \varepsilon/2 & \varepsilon_2 \end{bmatrix}$ in equation (A.6), where $\sigma_4 = k\sigma_1 = k\sigma = \varepsilon/S_{44}$ with $k = \frac{S_{11}}{S_{44}}$ is a real number, the deformation matrix is:

$$[\boldsymbol{F}] = \begin{bmatrix} \varepsilon + 1 & 0 & 0 \\ 0 & \varepsilon_2 + 1 & \varepsilon/2 \\ 0 & \varepsilon/2 & \varepsilon_2 + 1 \end{bmatrix} \tag{A.27}$$

Hence,

$$\boldsymbol{J} = |\det \boldsymbol{F}| = (\varepsilon + 1) \cdot [(\varepsilon_2 + 1)^2 - \varepsilon^2/4] \tag{A.28}$$

The right Cauchy-Green deformation tensor

$$[\boldsymbol{C}] = [\boldsymbol{F}]^{\boldsymbol{T}} \cdot [\boldsymbol{F}] = \begin{bmatrix} (\varepsilon + 1)^2 & 0 & 0 \\ 0 & (\varepsilon_2 + 1)^2 + \varepsilon^2/4 & \varepsilon(\varepsilon_2 + 1) \\ 0 & \varepsilon(\varepsilon_2 + 1) & (\varepsilon_2 + 1)^2 + \varepsilon^2/4 \end{bmatrix} \tag{A.29}$$

Then, the Almansi-Lagrange strain tensor:

$$[\boldsymbol{e}] = \frac{1}{2}\left([\boldsymbol{I}] - [\boldsymbol{C}^{-1}]\right) = \frac{1}{2}\begin{bmatrix} 1 - \dfrac{1}{(\varepsilon + 1)^2} & 0 & 0 \\ 0 & 1 - \dfrac{(\varepsilon_2 + 1)^2 + \varepsilon^2/4}{D^2} & \dfrac{\varepsilon(\varepsilon_2 + 1)}{D^2} \\ 0 & \dfrac{\varepsilon(\varepsilon_2 + 1)}{D^2} & 1 - \dfrac{(\varepsilon_2 + 1)^2 + \varepsilon^2/4}{D^2} \end{bmatrix} \tag{A.30}$$

With $D = (\varepsilon_2 + 1)^2 - \varepsilon^2/4$.

And the second Poila-Kirchhoff strain tensor:

$$\begin{aligned}[\widetilde{\boldsymbol{T}}] &= \boldsymbol{J} \cdot [\boldsymbol{F}^{-1}] \cdot [\boldsymbol{T}] \cdot [\boldsymbol{F}^{-1}]^{\boldsymbol{T}} \\ &= (\varepsilon + 1)\sigma \cdot D \cdot \begin{bmatrix} \dfrac{1}{(\varepsilon + 1)^2} & 0 & 0 \\ 0 & \dfrac{-k\varepsilon(\varepsilon_2 + 1)}{D^2} & \dfrac{k((\varepsilon_2 + 1)^2 + \varepsilon^2/4)}{D^2} \\ 0 & \dfrac{k((\varepsilon_2 + 1)^2 + \varepsilon^2/4)}{D^2} & \dfrac{-k\varepsilon(\varepsilon_2 + 1)}{D^2} \end{bmatrix}\end{aligned} \tag{A.31}$$

Then the stored elastic energy in the crystal is estimated as follow:

$$f_{el}^{l} = Y_{111}^{l} \cdot \varepsilon^2 \tag{A.32}$$

with:

$$Y_{111}^{l} = \frac{1}{4}\frac{\varepsilon^2}{S_{11}} \cdot \frac{(\varepsilon + 2)D}{(\varepsilon + 1)^3} + \frac{1}{2}\frac{\varepsilon^2}{S_{44}}\frac{(\varepsilon + 1)(\varepsilon_2 + 1)}{D}\left[\left(\frac{2(\varepsilon_2 + 1)^2 + \varepsilon^2/2}{D^2} - 1\right)\right] \tag{A.33}$$

Appendix B: Calculation preferences

B.1 Calculation of η

As mentioned earlier (equation A.14), $\eta = \frac{1}{a}\frac{\partial a}{\partial x}$ is the rate of change of the lattice constants with composition. If $\frac{\partial a}{\partial x}$ is a constant over the entire composition range, it is called Vegard's coefficient. From the definition, it is easy to see that η is not a constant. Actually, in studies[3, 5, 6], η is defined to be equal to $\eta = \frac{1}{a_0} * \frac{\partial a}{\partial x}$ with a_0 is the lattice constant of the interested solid solution. The definition of η makes it become flexible by changing the unit of composition and the reference value a_0. However, in many studies reporting the calculation of coherent miscibility gap using Cahn's approach, η is considered as a constant. The unclear explaination of the calculation procedures of η value makes us confused. Because η is an important parameter in the calculation of coherent miscibility gap, in this study, we would like to first, consider η as a paramenter represent the lattice misfit between two lattices and second, explain how η alters with changing reference value a_0. The variation of η corresponding to the reference a_0 of either two pure compounds is not significant, e.g. ~6% in Al-Zn system. However, in order to avoid any consfusion in the calculation of η value, we consider two kind of η:

- Constant η should be suitable for the solid solution which obeys Vegard's rule or slightly deviates from Vegard's rule:

$$\eta = \frac{1}{a_0} * \frac{\partial a}{\partial x} = \left| \frac{1}{a_{A_{0.5}B}} * \frac{a_A - a_{A_{0.5}B}}{0.5} \right| = 2 \left| \frac{a_A - a_B}{a_A + a_B} \right| \tag{B.1}$$

where A and B are two pure which form the solid solution A_xB. The absolute value sign is used since only the magnitude of η is important.

- Composition-dependent η is appropriate for the solid solution which significantly deviates from Vegard's rule:

$$\eta(x) = \frac{1}{a(x)} * \frac{\partial a}{\partial x} \tag{B.2}$$

B.2 Temperature dependence of physical properties

For calculating the coherent miscibility gap and spinodal, we need to use some physical properties such as lattice parameters, molar volumes, elastic constants, etc. Clearly, they are temperature dependent. In this study, for showing the effect of temperature dependence of physical properties in our calculation of coherent miscibility gap of various system, two kinds of calculation namely calculation of coherent miscibility gap with or without temperature effect are performed:

- For calculation without temperature effect, all physical properties are taken from available data at or near room temperature.
- For calculation with temperature effect, all physical properties need to be calculated at different temperatures. The elastic constants are considered as functions of temperature by fitting available data of elastic constants with temperature. If there are available data of lattice parameters with temperature, we could do the fitting process to obtain a temperature dependent function of lattice parameters. If no data is available, the lattice parameters are considered as a function of thermal expansion as follow:

$$a = a^* \cdot \left(1 + \alpha \cdot (T - T^*)\right) \tag{B.3}$$

with a and a^* are the lattice constants at temeprature T and T^*, respectively; α is the thermal expansion coefficient. Then, η, V_m, etc. are calculated correspondingly.

B.3 Physical properties of the solid solution

The experimental data of elastic constants, lattice parameters of the solid solution are not always available in all systems. If experimental or modeled data are available, it is easy to fit the elastic constants, lattice parameters of the solid solution as a function of its compositions. For many cases, the function is linear. In our following case study, we would do the fitting of the reported physical properties with the composition of the solid solution. However, if there is no reported data available, we assume that elastic constants, lattice parameters of the solid solution are linearly dependent on its compositions.

Appendix C: Elastic properties of materials

In this study, the values of elastic constants near room temperature are used in the calculation without temperature effect of elastic properties. The expression of elastic constants as a function of temperature is resulted from fitting the reported elastic constants at various temperatures.

Notice that in order to estimate the elastic constants of the FCC Al-Zn solid solution, we first calculated the elastic constants of the metastable FCC Zinc as no experimental data are reported in literature. The elastic constants were calculated *Ab initio* via Density Functional Theory (DFT). In the present study, DFT are based on the Plane-Wave basis sets and are done using the *Vienna Ab initio Simulation Package* (VASP)[7-10] using periodic boundary conditions. The Projected Augmented Wave (PAW) approach is employed to represent the core electrons.[11, 12] Generalized Gradient Approximation (GGA) parameterized by Perdew, Burke and Ernzerhof (PBE)[13, 14] was used as the exchange-correlation functional. Plane-Wave kinetic cut-of energy of 520 eV and Monkhorst Pack grid of 13×13×13 dimension to sample the Brillouin zone with a first order Methfessel-Paxton smearing parameter σ of 0.02 eV are used to ensure the force and energy convergence criterion are better than 0.02 eV/Å and 0.01 meV, respectively. The procedure to determine the elastic constants C_{ij} is well established and is detailed in our prior publications.[15-17] Basically, it consists in calculating the energy difference between the equilibrium lattice $\boldsymbol{R}$ and distorted lattice $\boldsymbol{R}'$, by applying very small strains (ε) in each crystallographic direction, in order to make sure we stay within the elastic domain. The relation between the equilibrium and distorted lattice is linear and defined as: $\boldsymbol{R}' = \boldsymbol{R}\boldsymbol{D}(\varepsilon)$ where $\boldsymbol{D}$ is the distortion matrix. For the FCC structure, there are 3 independent elastic constants and many distortions matrices can be found in Ravindran et al.[18] C_{ij} are obtained by fitting the 3 energy curves $El(\varepsilon)$ by a second order polynomial.

Table C1: List of elastic properties collected from the literature

Material/ Structure	T [K]	Elastic constants			Reference
		C_{11} [GPa]	C_{12} [GPa]	C_{44} [GPa]	
Al	293	106.49	60.39	28.28	Gerlich & Fisher[19]
	0-925	$117.6243 - 0.0392 \cdot T$	$63.0013 - 0.0094 \cdot T$	$32.5909 - 0.0151 \cdot T$	Kamm & Alers[20] and Gerlich & Fisher[19]
Ag	300	124	94	46.5	Chang & Himmel[21]
	300-800	$134.6136 - 0.0350 \cdot T$	$99.6409 - 0.0192 \cdot T$	$52.2209 + 0.0191 \cdot T$	Chang & Himmel[21]
Au	300	158.24	131.56	34.92	Cagin et al.[22]
	300-1000	$185.92 - 0.088 \cdot T$	$151.97 - 0.0648 \cdot T$	$42.881 - 0.0257 \cdot T$	Cagin et al.[22]
Co (FCC)	710	223	186	110	Strausse et al.[23]
Cu	300	170.0	122.5	75.8	Chang & Himmel[21]
	300-800	$181.7955 - 0.0405 \cdot T$	$128.5000 - 0.0200 \cdot T$	$83.9645 - 0.0271 \cdot T$	Chang & Himmel[21]
Ni	300	250.80	150.00	123.50	Alers et al.[24]
	280-760	$270.1 - 0.0625 \cdot T$	$152.52 - 0.0075 \cdot T$	$135.38 - 0.0392 \cdot T$	
Pt	300	289.63	239.55	65.07	Cagin et al.[22]
	300-1500	$319.2 - 0.0926 \cdot T$	$261.43 - 0.0686 \cdot T$	$73.223 - 0.0271 \cdot T$	Cagin et al.[22]
Zn (FCC)	0	106	70	11	Our first priciple calculation
CaO	300	220.53	57.67	80.3	Oda et al.[25]

	300-1200	$234.39 - 0.0471 \cdot T$	$57.4884 + 0.0015 \cdot T$	$82.4079 - 0.0075 \cdot T$	Oda et al.[25]
MgO	273	298.96	96.42	157.13	Isaak et al.[26]
	300-1800	$314.7003 - 0.0597 \cdot T$	$96.5851 - 0.0008 \cdot T$	$161.0125 - 0.0151 \cdot T$	Sumino et al.[27] and Isaak et al.[26]
KCl	298	40.69	7.11	6.31	Slagle & McKinstry[28]
	298-1073	$41.54 - 31.88 \cdot 10^{-3} \cdot (T - 273.15) + 3.47 \cdot 10^{-6} \cdot (T - 273.15)^2$	$6.96 + 4.36 \cdot 10^{-3} \cdot (T - 273.15) - 4.23 \cdot 10^{-6} \cdot (T - 273.15)^2$	$6.34 - 1.2 \cdot 10^{-3} \cdot (T - 273.15) - 0.88 \cdot 10^{-6} \cdot (T - 273.15)^2$	Slagle & McKinstry[28]
NaCl	298	49.47	12.88	12.87	Slagle & McKinstry[28]
	298-1073	$50.39 - 37 \cdot 10^{-3} \cdot (T - 273.15) + 4.36 \cdot 10^{-6} \cdot (T - 273.15)^2$	$12.69 + 12.78 \cdot 10^{-3} \cdot (T - 273.15) + 12.92 \cdot 10^{-6} \cdot (T - 273.15)^2$	$12.86 - 3.08 \cdot 10^{-3} \cdot (T - 273.15) - 1.58 \cdot 10^{-6} \cdot (T - 273.15)^2$	Slagle & McKinstry[28]
$Na_{1-x}K_xCl$	298	$C_{11}^{NaCl}(1-x) + C_{11}^{KCl}x - 25x(1-x)$	$C_{12}^{NaCl}(1-x) + C_{12}^{KCl}x - 11x(1-x)$	$C_{44}^{NaCl}(1-x) + C_{44}^{KCl}x - 10x(1-x)$	Botaki et al.[29]
	298-1073	$C_{11}^{NaCl}(1-x) + C_{11}^{KCl}x - 25x(1-x)$	$C_{12}^{NaCl}(1-x) + C_{12}^{KCl}x - 13x(1-x)$	$C_{44}^{NaCl}(1-x) + C_{44}^{KCl}x - (14.394 - 0.0147 \cdot T)x(1-x)$	Botaki et al.[29]

Appendix D: Lattice parameters, molar volume and thermal expansion coefficients

Table D1: List of lattice parameters and molar volume used in this study

Material/ Structure	Lattice parameter [m]	Molar volume [m^3/mol]	Reference
Al	$403 \cdot 10^{-12}$	$9.78189 \cdot 10^{-6}$	Kittel[30]
Ag	$408.57 \cdot 10^{-12}$	$10.2696 \cdot 10^{-6}$	Subramania & Perepezko[31]
Au	$407.84 \cdot 10^{-12}$	$1.0215 \cdot 10^{-5}$	Lubarda[32]
Co	$354.8 \cdot 10^{-12}$	$6.7252 \cdot 10^{-6}$	Cerda et al.[33]
Cu	$361.46 \cdot 10^{-12}$	$7.111 \cdot 10^{-6}$	Subramania & Perepezko[31]
Ni	$352.4 \cdot 10^{-12}$	$6.5888 \cdot 10^{-6}$	Lubarda[32]

Pt	$392.38 \cdot 10^{-12}$	$9.0951 \cdot 10^{-6}$	Arblaster[34]
Zn (FCC)	$3.79 \cdot 10^{-10}$	$8.65149 \cdot 10^{-6}$	Muller et al.[35]
CaO	$4.811 \cdot 10^{-10}$	$16.764 \cdot 10^{-6}$	Fiquet et al.[36]
	$(4.7866 + 7.6 \cdot 10^{-5} \cdot T) \cdot 10^{-10}$		Fiquet et al.[36]
MgO	$4.210 \cdot 10^{-10}$	$11.228 \cdot 10^{-6}$	Fiquet et al.[36]
	$(4.180459 + 7.3 \cdot 10^{-5} \cdot T) \cdot 10^{-10}$		Fiquet et al.[36]
KCl	$6.2916 \cdot 10^{-10}$	$37.5004 \cdot 10^{-6}$	Barrett & Wallace[37]
NaCl	$5.64 \cdot 10^{-10}$	$27.0141 \cdot 10^{-6}$	Barrett & Wallace[37]

Table D2: Thermal expansion coefficient of substances

Material/ Structure	Linear thermal expansion coefficient [10^{-6}/K]	Reference
Al	23.1	Cohen et al.[38]
Ag	18.9	Cohen et al.[38]
Au	14.2	Cohen et al.[38]
Co (HCP)	13	Cohen et al.[38]
Cu	16.5	Cohen et al.[38]
Ni	13.4	Cohen et al.[38]
Pt	8.8	Cohen et al.[38]
Zn (HCP)	30.2	Cohen et al.[38]
KCl	36.2	Pathak & Vasavada[39]
NaCl	39.8	Pathak & Vasavada[39]

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