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# Excess entropy of mixing for binary square-well fluid in the mean spherical approximation: Application to liquid alkali-metal alloys

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ABSTRACT

The expression for the entropy of binary square-well (SW) mixture is derived in the framework of the semi-analytical approach [J. Non-Cryst. Solids 353 (2007) 1798] for the mean spherical approximation. This expression is applied to calculate the concentration dependencies of the excess entropy of mixing for liquid Na-K and Na-Cs alloys at $T = 373$ K. It is shown that the SW model allows to achieve a better agreement with experiment than the hard-sphere model with the same values of hard-core parameters.



## 1. Introduction

Different types of fluids can be described by means of the square-well (SW) model: non-polar molecular fluids [1–3], colloids [4–7], aqueous electrolyte solutions [8,9], polymers [10–12] and polar and associating compounds, including water [13,14] and metal liquids [15–21] (for last, the SW model was used recently as a reference system also [22–24]).

For liquid metals, the SW model is able to describe the structure factor with low-lying shoulder on the high-angle side of the first peak [15]. In liquid metal binary alloys, this model can describe different deviations from the ideal mixing such as tendencies to chemical short-range ordering [18] or to phase separation [19].

In majority of works where the SW model is applied to metal state, the random phase approximation (RPA) [25–27] is used. Only recently, going beyond the framework of the RPA was implemented in this field [20,21] by using the mean spherical approximation (MSA) [28] for which the semi-analytical (SA) procedure suggested by Dubinin et al. [29] was conducted. Notice that the MSA-SA procedure reproduces explicitly the numerical MSA results obtained by solving the Ornstein–Zernike integral equation [30] both for a pure [31] and for binary [32] SW fluid at an appropriate number of coefficients in the expansion suggested by Dubinin et al. [29]. In the study of Dubinin et al. [21], the SW-MSA-SA was used to study the partial structure factors of liquid equiatomic Na-K alloy.

Here, we derive the MSA-SA expression for the entropy of binary SW mixture (earlier, expressions for the entropy of pure SW fluid were derived within the RPA [22] and within the MSA-SA [24]) and estimate its usefulness for liquid metal alloys on the example of Na-K and Na-Cs systems.

These systems are interesting for consideration since their entropies of mixing very little deviate from the entropy of the ideal solution, $S_{id}$. In that case, the excess entropy of mixing, $\Delta S^{ex}$, is very small and sensitive to the method of calculation. Consequently, this quantity namely is chosen here for investigation.

## 2. Theory

For a binary alloy, $\Delta S^{ex}$ is expressed as follows:

$$\Delta S^{ex} = S^{bin} - \sum_{i=1}^{2} c_i S_i^{pure} - S_{id}, \tag{1}$$

where $S^{bin}$ is the entropy of binary alloy, $S_i^{pure}$ is the entropy of the $i$th-kind pure substance at the same absolute temperature, $T$ (further, we neglect indexes "pure" and "i," denoting the thermodynamic quantities of pure substances) and $c_i$ is the concentration of the $i$th component in the alloy. The entropy of the ideal solution is calculated as follows:

$$S_{id} = -k_B(c_1 \ln c_1 + c_2 \ln c_2). \tag{2}$$

Consider a one-component SW fluid that is described by the following three-parameter model pair potential:

$$\varphi_{SW}(r) = \begin{cases} \infty, & r<\sigma \\ \phi_{SW}(r), & r \geq \sigma \end{cases}, \tag{3}$$

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where $\sigma$ is the diameter of the hard core (HC);

$$\phi_{SW}(r) = \begin{cases} 0, & r<\sigma \\ \varepsilon, & \sigma \le r<\lambda\sigma; \\ 0, & r\ge\lambda\sigma \end{cases} \tag{4}$$

$\varepsilon$ and $\sigma(\lambda - 1)$ are the depth and width of the square well, respectively.

The entropy of such a fluid can be expressed as follows:

$$S_{SW} = S_{HS} + \Delta S_{SW} = S_{IG} + \Delta S_{HS} + \Delta S_{SW}, \tag{5}$$

where $S_{HS}$ is the entropy within the hard-sphere (HS) model, $\Delta S_{SW}$ is the contribution due to the difference between SW and HS entropies and $S_{IG}$ is the entropy of the ideal gas (hereafter, all thermodynamic quantities will be written in atomic units (a.u.) per atom), calculated as follows:

$$S_{IG} = k_B\left[\frac{5}{2} + \ln\left(\frac{1}{\rho}\left[\frac{k_B T m}{2\pi}\right]^{\frac{3}{2}}\right)\right]. \tag{6}$$

Here, $k_B$ is the Boltzmann constant, $\rho$ is the mean number density and $m$ is the atomic mass.

$\Delta S_{SW}$ in the framework of the MSA-SA was obtained by Dubinin et al. [24]:

$$\Delta S_{SW\text{-}MSA\text{-}SA} = \frac{k_B}{4\pi^2\rho}\int_0^\infty (\ln[(1-\rho\Delta c(q))\chi_{SW-MSA\text{-}SA}(q)] - (1-\rho\Delta c(q))\chi_{SW-MSA\text{-}SA}(q) + 1)q^2 dq \tag{7}$$

where $\chi(q)$ is the structure factor, calculated as follows:

$$\chi_{SW\text{-}MSA\text{-}SA}(q) = \frac{1}{1-\rho\Delta c(q) + \beta\rho\phi_{SW}(q)}; \tag{8}$$

$$\Delta c(q) = \left(\frac{4\pi}{q^3}\right)\left\{\sum_{m=1}^{n+2} x^{2-m}\frac{\partial^m \sin(x)}{\partial x^m}\sum_{l=0}^{n} b_l \prod_{k=0}^{m-2}(l+1-k) + \sum_{m=1}^{[(n+1)/2]}\frac{(-1)^{m+1}(2m)!b_{(2m-1)}}{x^{2m-1}}\right\}. \tag{9}$$

Here,

$$\phi_{SW}(q) = 4\pi\varepsilon[\sin(\lambda x) - \sin(x) - \lambda x\cos(\lambda x) + x\cos(x)]/q^3; \tag{10}$$

$\beta = (k_B T)^{-1}$, $x = q\sigma$, $[a]$ is the integral part of $a$, $b_m$ is the coefficient determined numerically from the condition that the pair correlation function, $g(r)$, must be equal to zero inside the HC.

To obtain Eq. (7), we used the following thermodynamic relation:

$$\left(\frac{\partial S}{\partial T}\right)_\rho = \frac{1}{T}\left(\frac{\partial E}{\partial T}\right)_\rho, \tag{11}$$

where $E$ is the internal energy.

For the SW fluid, Eq. (11) leads to the following expression [24]:

$$\left(\frac{\partial(\Delta S_{SW})}{\partial T}\right)_\rho = \frac{1}{T}\left(\frac{\partial U_{SW}}{\partial T}\right)_\rho, \tag{12}$$

where $U_{SW}$ is the SW potential energy:

$$U_{SW} = 2\pi\rho\int_0^\infty \varphi_{SW}(r)g_{SW}(r)r^2 dr = 2\pi\rho\int_\sigma^{\lambda\sigma}\phi_{SW}(r)g_{SW}(r)r^2 dr. \tag{13}$$

For subsequent operations, $U_{SW}$ within the MSA-SA form in the wave space will be used:

$$U_{SW\text{-}MSA\text{-}SA} = \frac{2}{3}\pi\rho\sigma^3\varepsilon\left(\lambda^3-1\right) + \frac{1}{4\pi^2}\int_0^\infty [\chi_{SW\text{-}MSA\text{-}SA}(q)-1]\phi_{SW}(q)q^2 dq. \tag{14}$$

For the binary SW mixture, Eqs. (3) and (4) are being transformed to the following expressions, respectively:

$$\varphi_{ijSW}(r) = \begin{cases} \infty, & r<\sigma_{ij} \\ \phi_{ijSW}(r), & r\ge\sigma_{ij} \end{cases}, \tag{15}$$

where $\sigma_{ij}$, $\varepsilon_{ij}$ and $\lambda_{ij}$ are the partial SW parameters ($i, j = 1, 2$);

$$\phi_{ijSW}(r) = \begin{cases} 0, & r<\sigma_{ij} \\ \varepsilon_{ij}, & \sigma_{ij}\le r<\lambda_{ij}\sigma_{ij} \\ 0, & r\ge\lambda_{ij}\sigma_{ij} \end{cases}. \tag{16}$$

The SW entropy of two-component fluid is written as follows:

$$S_{SW}^{bin} = S_{IG}^{bin} + S_{id} + \Delta S_{HS}^{bin} + \Delta S_{SW}^{bin}, \tag{17}$$

where

$$S_{IG}^{bin} = k_B\left[\frac{5}{2} + \ln\left(\frac{1}{\rho^{bin}}\left[\frac{k_B T m_1^{c_1} m_2^{c_2}}{2\pi}\right]^{\frac{3}{2}}\right)\right]. \tag{18}$$

To obtain $\Delta S_{SW}^{bin}$, we use the way similar to that for the one-component case, i.e., rewrite Eq. (12) as follows:

$$\left(\frac{\partial\left(\Delta S_{SW}^{bin}\right)}{\partial T}\right)_{\rho^{bin}} = \frac{1}{T}\left(\frac{\partial U_{SW}^{bin}}{\partial T}\right)_{\rho^{bin}}, \tag{19}$$

where

$$U_{SW}^{bin} = \frac{2}{3}\pi\rho^{bin}\sum_{i,j=1}^{2} c_i c_j \sigma_{ij}^3\varepsilon_{ij}\left(\lambda_{ij}^3-1\right) + \frac{1}{4\pi^2}\sum_{i,j=1}^{2}\sqrt{c_i c_j}\int_0^\infty\left[\chi_{ijSW}(q)-\delta_{ij}\right]\phi_{ijSW}(q)q^2 dq. \tag{20}$$

Here, $\chi_{ij}(q)$ is the partial structure factor in the form of Ashcroft and Langreth [33]:

$$\chi_{ii}(q) = \frac{1-c_j\rho^{bin}c_{jj}(q)}{[1-c_1\rho^{bin}c_{11}(q)][1-c_2\rho^{bin}c_{22}(q)] - c_1c_2\rho^{bin^2}c_{12}^2(q)}, \tag{21}$$

$$\chi_{12}(q) = \frac{\sqrt{c_1c_2}\rho^{bin}c_{12}(q)}{[1-c_1\rho^{bin}c_{11}(q)][1-c_2\rho^{bin}c_{22}(q)] - c_1c_2\rho^{bin^2}c_{12}^2(q)}, \tag{22}$$

where $c_{ij}(r)$ is the partial direct correlation function. Within the SW-MSA-SA, this characteristic is written as follows:

$$c_{ijSW\text{-}MSA\text{-}SA}(q) = -\beta\phi_{ijSW}(q) + \Delta c_{ij}(q), \tag{23}$$

**Table 1**
Values of the SW parameters used for the calculation.

| | σ (a.u.) | ε (a.u.) | λ |
|---|---|---|---|
| Na | 6.2544 | −0.00100 | 1.435 |
| K | 7.7038 | −0.00025 | 1.479 |
| Cs | 8.792 | −0.00025 | 1.461 |

where

$$\Delta c_{ii}(q) = \left(\frac{4\pi}{q^3}\right)\left\{\sum_{m=1}^{n+2} x_{ii}^{2-m}\frac{\partial^m \sin(x_{ii})}{\partial x_{ii}^m}\sum_{l=0}^{n} b_{iil}\prod_{k=0}^{m-2}(l+1-k) + \sum_{m=1}^{[(n+1)/2]}\frac{(-1)^{m+1}(2m)!b_{ii(2m-1)}}{x_{ii}^{2m-1}}\right\} \quad (24)$$

$$\Delta c_{12}(q) = \left(\frac{4\pi}{q^3}\right)\left\{\sum_{m=1}^{n+2} x_{11}^{2-m}\frac{\partial^m \sin(x_{12})}{\partial x_{12}^m}\sum_{l=0}^{n} b_{12l}\prod_{k=0}^{m-2}(l+1-k) + y_{12}b_{120}\cos(x_{12}) + \sum_{m=1}^{n}\frac{(m+1)!b_{12m}}{x_{11}^m}\frac{\partial^m \sin(y_{12})}{\partial y_{12}^m}\right\} \quad (25)$$

where $x_{ij} = q\sigma_{ij}$, $y_{12} = q(\sigma_{22}-\sigma_{11})/2$ at $\sigma_{22} > \sigma_{11}$, $b_{ijm}$ are coefficients determined by a similar way as in the case of the one-component fluid by means to satisfy the following conditions:

$$g_{ij}(r) = 0, \quad r<\sigma_{ij}. \quad (26)$$

In the framework of the MSA-SA, Eqs. (19) and (20) lead to the following expression for $\Delta S_{SW}^{bin}$:

$$\Delta S_{SW\text{-}MSA\text{-}SA}^{bin} = \frac{k_B}{4\pi^2}\sum_{i=1}^{2} c_i\int_0^\infty dq q^2 \phi_{iiSW}(q)\int\frac{\partial \chi_{iiSW-MSA\text{-}SA}(q)}{\partial\beta}\beta d\beta + \frac{k_B\sqrt{c_1c_2}}{2\pi^2}\int_0^\infty dq q^2\phi_{12SW}(q)\int\frac{\partial\chi_{12SW-MSA\text{-}SA}(q)}{\partial\beta}\beta d\beta \quad (27)$$

After some transformations, Eq. (27) can be rewritten as follows:

$$\Delta S_{SW\text{-}MSA\text{-}SA}^{bin} = \frac{k_B}{4\pi^2}\int_0^\infty dq q^2\left\{\beta\sum_{i,j=1}^{2}\sqrt{c_ic_j}\phi_{ijSW}(q)\chi_{ijSW-MSA}(q) - \frac{1}{\rho^{bin}}\ln\frac{h(q)+f(q)\beta+g(q)\beta^2}{h(q)}\right\}, \quad (28)$$

where

$$\begin{aligned} h(q) &= 1-\rho^{bin}\sum_{i=1}^{2}c_i\Delta c_{ii}(q) + c_1c_2\rho^{bin2}\left[\Delta c_{11}(q)\Delta c_{22}(q)-\Delta c_{12}^2(q)\right]; f(q)\\ &= \rho^{bin}\sum_{i=1}^{2}c_i\phi_{iiSW}(q) - c_1c_2\rho^{bin2}\left[\sum_{i=1}^{2}\Delta c_{ii}(q)\phi_{iiSW}(q) - 2\Delta c_{12}(q)\phi_{12SW}(q)\right]; g(q)\\ &= c_1c_2\rho^{bin2}\left[\phi_{11SW}(q)\phi_{22SW}(q)+\phi_{12SW}^2(q)\right]. \end{aligned} \quad (29)$$

**Table 2**
Values of the mean atomic volumes (in a.u.) used for the calculation.

| $c_{Na}$ | 0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $\Omega_{Na-K}^{bin}$ | 559 | 528 | 498 | 469 | 442 | 415 | 389 | 364 | 340 | 316 | 292 |
| $\Omega_{Na-Cs}^{bin}$ | 871 | 797 | 729 | 666 | 607 | 550 | 496 | 444 | 392 | 342 | 292 |

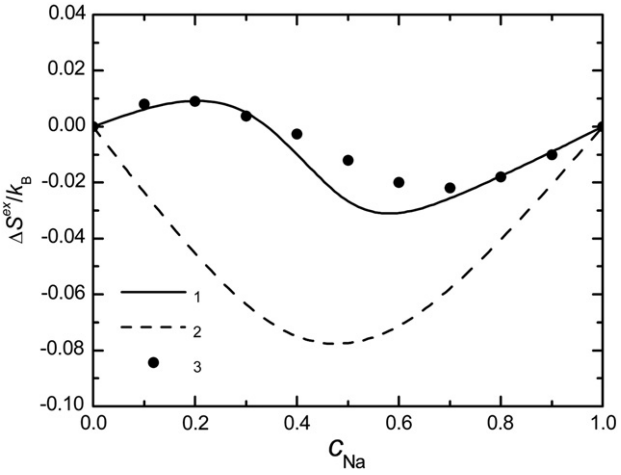


**Fig. 1.** Concentration dependency of the excess entropy of mixing in liquid Na-K alloy at $T = 373$ K (1—SW calculation; 2—HS calculation; 3—experiment [37]).

## 3. Details of calculations

Both $\Delta S_{HS}$ and $\Delta S_{HS}^{bin}$ are used in the form obtained from the compressibility equation following the work [34]:

$$\Delta S_{HS} = k_B\left[\ln(1-\eta)+\frac{3}{2}\left(1-\frac{1}{(1-\eta)^2}\right)\right], \quad (30)$$

$$\Delta S_{HS}^{bin} = k_B\left[\ln\left(1-\eta^{bin}\right)+\frac{3}{2}\left(1-\frac{1}{\left(1-\eta^{bin}\right)^2}\right) + \pi c_1c(\sigma_{11}-\sigma_{22})^2\frac{12(\sigma_{11}+\sigma_{22})-\pi\rho\left(c_1\sigma_{11}^4+c_2\sigma_{22}^4\right)}{24\left(1-\eta^{bin}\right)^2}\right] \quad (31)$$

where $\eta = (\pi\rho\sigma^3/6)$ and $\eta^{bin} = \frac{\pi\rho^{bin}}{6}\sum_{i=1}^{2}c_i\sigma_{ii}^3$.

The SW binary model is taken within the traditional additive form (see, for example, [17]), where $\sigma_{12} = (\sigma_{11}+\sigma_{22})/2$; $\varepsilon_{12} = -\sqrt{\varepsilon_{11}\varepsilon_{22}}$; $\lambda_{12} = (\lambda_{11}\sigma_{11}+\lambda_{22}\sigma_{22})/(\sigma_{11}+\sigma_{22})$.

In Eqs. (9), (24) and (25), we take $n = 5$, which is sufficient for an accuracy better than 0.1%.

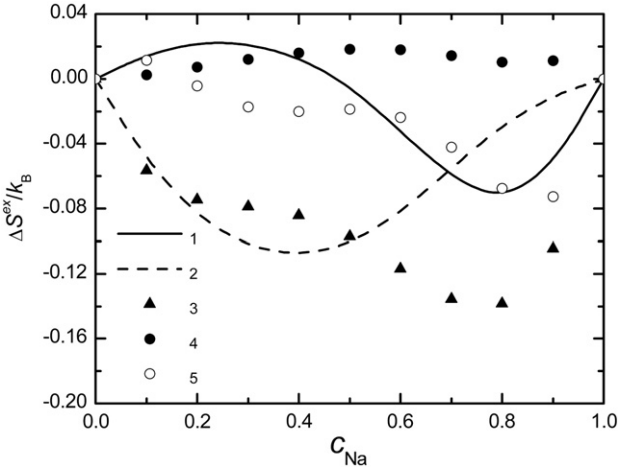


**Fig. 2.** Concentration dependency of the excess entropy of mixing in liquid Na-Cs alloy at $T = 373$ K (1—SW calculation; 2—HS calculation; 3—experiment [38]; 4—experiment [39]; 5—experiment [40]).

The simplex method is used to solve equation $g(r) = 0$ at $r < \sigma$ for a pure fluid and Eq. (26) for a binary mixture.

## 4. Results and discussion

The expression obtained is applied to study Na-K and Na-Cs liquid alloys at $T = 373$ K. Input data for pure Na, K and Cs at the aforementioned temperature are given in Table 1. For $\sigma$, we take values obtained earlier by using the variational method with HS reference system realized for an effective pair potential constructed in the framework of the pseudopotential theory [35]. At fixed $\sigma$ for each metal, we define $\varepsilon$ and $\lambda$ as adjustable parameters by fitting the calculated structure factor with respect to experiment [36]. Partial parameters with indexes *ii* are assumed equal to parameters of corresponding pure metal. The mean atomic volumes of alloys under consideration, $\Omega^{\text{bin}} = 1/\rho^{\text{bin}}$, at different alloy compositions are taken from Dubinin et al. [35] and listed in Table 2.

The calculated concentration dependencies of the excess entropy of mixing for the Na-K and Na-Cs alloys are shown in Figs. 1 and 2, respectively. The curves obtained are compared with HS results (at $\varepsilon_{\text{Na}} = \varepsilon_{\text{K}} = \varepsilon_{\text{Cs}} = 0$) and with experimental data [37–40].

It can be seen from Figs. 1 and 2 that an additional contribution to the HS entropy due to the SW attraction gives an improvement of calculated excess entropy of mixing. Besides, it is defined that a good quantitative description of the entropy of binary alloy can be achieved at the same values of the SW parameters that lead to a good description of the structure characteristics in corresponding pure liquid metals.

## 5. Conclusion

In the present work, the MSA-SA expression for the entropy of binary SW mixture has been derived. The high usefulness of this expression is shown on the example of the excess entropy of mixing in liquid Na-K and Na-Cs systems at different component concentrations.

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