Variational Calculations for Liquid Na-Cs Alloy

I. The Isothermal Compressibility

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Abstract

The concentration dependency of the isothermal compressibility of the Na-Cs liquid alloy at $T=373K$ is calculated by the variational method with hard-sphere reference system. The local Animalu-Heine model pseudopotential and Toigo-Woodruff exchange-correlation function are used for the calculation. Very good agreement with experimental data is achieved.

Keywords: Variational method, pseudopotential theory, liquid binary metal alloy, isothermal compressibility

The isothermal compressibility, $\chi_T$, is the quantity inversely to the bulk modulus, $B_T$:

$$\chi_T = 1 / B_T,$$  \hspace{1cm} (1)

$$B_T = \Omega \left( \partial^2 F / \partial \Omega^2 \right)_F,$$  \hspace{1cm} (2)

where $\Omega$ is the mean atomic volume, $F$ – Helmholtz free energy, $T$ – temperature.

In present study, Eq. (2) is calculated numerically from $F$ obtained by the variational method of the thermodynamic perturbation theory [1] for each alloy composition under consideration. For application to liquid metal binary alloys the variational method was developed and described in detail by Umar et al. [2]. We use this approach in conjunction with the additional condition that the pressure must be equal to zero:
\begin{equation}
(\partial F / \partial \Omega)_{T, \sigma_j} = 0 ,
\end{equation}

where $\sigma_j$ is the partial diameter of the additive hard-sphere model, which is used here as a reference system; $i, j = 1, 2$.

The pseudopotential model is taken in the local approximation [3] of the Animalu-Heine (AH) form [4] with the following form-factor for the unscreened $i$-th kind ion, $\omega_{i\text{AH}(0)}(q)$ (in atomic units (a.u.)):

\begin{equation}
\omega_{i\text{AH}(0)}(q) = \frac{4\pi}{\Omega q^2} \left[ (A_i R_{Mi} - z) \cos(qR_{Mi}) - \frac{A_i R_{Mi} \sin(qR_{Mi})}{qR_{Mi}} \right] \exp \left[ -0.03 \left( \frac{q}{2k_F} \right)^4 \right] (4)
\end{equation}

where $z$ is the mean alloy valence, $k_F$ – Fermi wave vector, $A_i$ and $R_{Mi}$ – $i$-th component parameters taken the same as for the corresponding pure metal.

Table 1. Values of pseudopotential parameters [3] used as input data

<table>
<thead>
<tr>
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<th>$A$ (a.u.)</th>
<th>$R_M$ (a.u.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na</td>
<td>-0.1958</td>
<td>2.1148</td>
</tr>
<tr>
<td>Cs</td>
<td>-0.1838</td>
<td>3.8677</td>
</tr>
</tbody>
</table>

**Figure 1.** Isothermal compressibility of the liquid Na-Cs alloy at $T=373K$ (1 – our calculation; 2 – calculation of Lai et al. [7]; 3 – experiment [6]).
The Toigo-Woodruff approximation [5] is used to represent the exchange-correlation function.

Very good agreement with the experiment [6] is achieved for the concentration dependency of \( \chi_T \) (Fig. 1). Besides, Fig. 1 shows that a sufficiently simple local pseudopotential as used here can give better results than the non-local pseudopotential with high-order perturbation corrections which was used in [7].

References


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