The SW-RPA Self-Diffusion Coefficient
of Liquid Potassium

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Abstract

The self-diffusion coefficient of the liquid potassium at $T=337K$ is calculated in the square-well model within the random phase approximation. A good agreement with available experimental data is obtained.

Keywords: Square-well model, random phase approximation, self-diffusion coefficient, liquid metal

In our previous works [1, 2] the square-well (SW) model within the random phase approximation with the hard-sphere reference system had been successfully applied to study the structure factor, $S(q)$, and the self-diffusion coefficient, $D = (\beta \xi)^{-1}$ (where $\xi$ is the friction coefficient, $\beta = (k_B T)^{-1}$, $k_B$ - Boltzmann constant, $T$ - temperature), of liquid Na near the melting point. Here, this approach is used to calculate $D$ of the liquid K at the same condition.

The Davis-Palyvos [3] approach is used for this aim:

\[ \xi = \xi_h + \xi_s + \xi_{SH}, \]

where $\xi_h$ and $\xi_s$ are the contributions due to the hard and soft part of the pair interaction, respectively, $\xi_{SH}$ - the cross-correlation term:

\[ \xi_h = \frac{8}{3} \rho \sigma^2 g(\sigma)(\pi M / \beta)^{1/2}, \]

\[ \xi_s = -\frac{(\beta \pi M)^{1/2}}{12 \pi^2} \int_0^{\infty} [S(q) - 1 - 3] \phi(q) q^2 dq, \]

\[ \xi_{SH} = -\frac{1}{3} \rho g(\sigma)(\beta M / \pi)^{1/2} \int_0^{\infty} [q \cos(q \sigma) - \sin(q \sigma)] \phi(q) dq, \]
where $\rho$ is the mean atomic density (taken here from [4]), $\sigma$ - hard-core diameter, $g(r)$ - radial distribution function, $M$ - atomic mass, $\phi(q)$ - Fourier transform of the soft part of the pair potential. The SW model parameters for liquid K are defined by fitting the first peak of $S(q)$ with respect to the experimental one [5].

Calculated $D$ is compared with two experimental results (Table 1). Like the case of liquid Na [2], it can be seen that the SW model gives slightly overstated value of $D$ in comparison with experimental ones.

<table>
<thead>
<tr>
<th>$D \cdot 10^{-9}$ (m$^2$/s)</th>
<th>SW</th>
<th>Experiment [6]</th>
<th>Experiment [7]</th>
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<tbody>
<tr>
<td></td>
<td>4.54</td>
<td>3.76</td>
<td>3.59</td>
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</tbody>
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Table 1. Self-diffusion coefficient of liquid K at $T = 337$ K.

References


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