Self-Diffusion Coefficient of Liquid Lithium

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Abstract

The self-diffusion coefficient of the liquid lithium at $T=454$K 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

Earlier, the square-well (SW) model in the random phase approximation with the hard-sphere reference system had been successfully applied to study the self-diffusion coefficient, $D=(\beta \xi)^{-1}$ (where $\xi$ is the friction coefficient, $\beta=(k_BT)^{-1}$, $k_B$ - Boltzmann constant, $T$ - temperature), of liquid Na and K near their melting points [1, 2]. Here, this approach is used to calculate $D$ of the liquid Li at the same condition.

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

$$\xi = \xi_H + \xi_S + \xi_{SH}, \quad (1)$$

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:

$$\xi_H = \frac{8}{3} \rho \sigma^2 g(\sigma)(\pi M / \beta)^{1/2}, \quad (2)$$

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

$$\xi_{SH} = -\frac{1}{3} \rho g(\sigma)(\beta M / \pi)^{1/2} \int_0^\infty [q\sigma \cos(q\sigma) - \sin(q\sigma)]\phi(q) dq. \quad (4)$$
where $\rho$ is the mean atomic density (taken here from [4]), $\sigma$ - hard-core diameter, $g(r)$ - radial distribution function, $M$ - atomic mass, $S(q)$ - structure factor, $\phi(q)$ - Fourier transform of the soft part of the pair potential. The SW model parameters for liquid Li 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).

Table 1. Self-diffusion coefficient of liquid Li at $T = 454$ K.

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<td>$D \times 10^9$ (m$^2$/s)</td>
<td>7.95</td>
<td>6.80</td>
<td>5.98</td>
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It can be seen that the SW model gives slightly overstated value of $D$ in comparison with experimental ones, similar to the cases of liquid Na [1] and K [2].

References


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