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The SW-RPA and HS-PY Self-Diffusion Coefficients for Liquid Sodium

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Abstract

The self-diffusion coefficient of liquid sodium is calculated in the square-well (SW) model within the random phase approximation and in the hard-sphere (HS) model. It is found that the HS value obtained is significantly larger than both SW obtained and experimental values.

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

In our previous work [1] the square-well (SW) model within the random phase approximation (RPA) had been successfully applied to study the structure factor of liquid Na at T=373K. Here, this approach is used to calculate the self-diffusion coefficient, $D=(\beta\xi)^{-1}$ (where ξ is the friction coefficient, $\beta=(k_{\mathrm{B}}T)^{-1}$, k_{B} - Boltzmann constant, T - absolute temperature), of this metal at the same conditions.

The Davis-Palyvos [2] approach is used for this aim:

$$\xi=\xi_{\mathrm{H}}+\xi_{\mathrm{S}}+\xi_{\mathrm{SH}} \quad , \tag{1}$$

where ξ_{H} and ξ_{S} are the contributions due to the hard and soft part of the pair interaction, respectively, ξ_{SH} - the cross-correlation term:

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

$$\xi_{\mathrm{S}}=-\frac{(\beta\pi M)^{1/2}}{12\pi^{2}}\int_{0}^{\infty}[S(q)-1]\phi(q)\,q^{3}\mathrm{d}q \quad , \tag{3}$$

$$\xi_{\mathrm{SH}} = -\frac{1}{3}\rho\, g(\sigma)(\beta M/\pi)^{1/2}\int_0^\infty [q\sigma\cos(q\sigma) - \sin(q\sigma)]\phi(q)\,\mathrm{d}q \quad , \tag{4}$$

where ρ is the mean atomic density, σ - hard-core diameter, $g(r)$ - radial distribution function, M - atomic mass, $S(q)$ - structure factor, $\phi(q)$ - Fourier transform of the soft part of pair interaction. In the limit hard-sphere (HS) case $\xi = \xi_{\mathrm{H}}$, where $g(\sigma)$ can be calculated analytically by using the Percus-Yevick (PY) [3] solution obtained in works [4, 5].

Input data for ρ, σ, and SW width are taken here the same as in the work [1]. Among values that were used in [1] for the SW depth, the value giving a better agreement with experiment for the structure factor ($\beta\varepsilon = -0.6$) is chosen.

Results obtained show that the SW model is more realistic than the HS one.

Table 1. Self-diffusion coefficient of liquid sodium at T = 373K.

	HS	SW	Experiment [6]
$D \cdot 10^{-9}$ (m^2/s)	8.54	5.67	4.19

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