

# Helium in liquid alkali metals: solubility and nucleation

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The easiest reaction to produce in a fusion reactor involves deuterium and tritium, producing helium (He) and one neutron (n)[1]. While the first isotope is stable and naturally present in water, the second must be obtained as a product from neutron captures by any of the two natural lithium isotopes, <sup>6</sup>Li and <sup>7</sup>Li[2]. He is also a by-product of the last reactions and, due to its very low solubility in lithium[3], may nucleate and form bubbles.

We investigate the possible formation of those bubbles using the molecular dynamics method. A mixture of Li and He atoms is described by a Hamiltonian composed by the Belashchenko embedded atom model (BEAM)[4] for Li-Li interactions and the Toennies-Tang-Sheng potentials (TTS) [5] for Li-He and He-He pairs.

The solubility of He is studied using Li, Na, K, Rb and Cs in their liquid state as solvents. We use the set of BEAM+TTS for the 5 alkali metals. We compute the Henry's constant, which is the ratio between the saturation pressure and concentration, from the work related to insert a single solute atom to a pure alkali metal system,

$$k_H = p^{\text{sat}}/x^{\text{sat}} = \rho k_B T \exp\{\beta \Delta\mu^{\text{excess}}\}. \quad (1)$$

The excess chemical potential  $\Delta\mu^{\text{excess}}$  is determined increasing gradually a control parameter  $0 < \xi < 1$  that multiplies the alkali-He potential, and adding an artificial potential  $V_{\text{cav}}(r; \lambda) = Ae^{-r/B+\lambda}$  that creates a void space (cavity) among the solvent atoms. This procedure was proposed by Li et al. [6] and is required because of the divergent behaviour of TTS ( $V(r) \sim r^{-1}$  for  $r \rightarrow 0$ ) we need to ensure finite forces during the whole simulation. The excess chemical  $\Delta\mu^{\text{excess}}$  is the sum of the free energy change during the growth, insertion and shrinkage stages:

$$\begin{aligned} \Delta\mu^{\text{excess}} &= \int_{\lambda_1}^{\lambda_2} d\lambda \langle V_{\text{cav}}(\lambda) \rangle_{V_{\text{cav}}(\lambda)} \\ &+ \int_0^1 d\xi \langle V_{\text{He-X}} \rangle_{V_{\text{cav}}(\lambda_2) + \xi V_{\text{He-X}}} \\ &+ \int_{\lambda_2}^{\lambda_1} d\lambda \langle V_{\text{cav}}(\lambda) \rangle_{V_{\text{cav}}(\lambda) + V_{\text{He-X}}} \quad (2) \end{aligned}$$

Then, we compare the temperature dependence of  $k_H$  from the model against experimental data[3]. Both results are in very good agreement and, as observed in Fig. 1, the logarithm of  $k_H$  turns out to be inversely linear to the temperature.

The results of  $k_H$  are employed in the study of the nucleation of He in Li. Simulations lead to highly stable clusters of He even for small nuclei. The critical radius is estimated from the Gibbs free energy (see Fig. 2), obtained as a sum of a bulk and a surface term. The first includes the reported values of  $k_H$ , and the second is computed based on the Thompson et al. method[7]. Bubbles formed by more than 100 He atoms ( $\sim 6 \text{ \AA}$ ) are always stable.

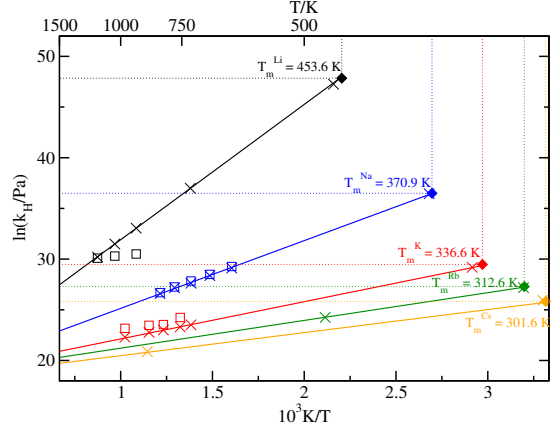


Fig. 1. Henry's constants for He in Li (black), Na (blue), K (red), Rb (green) and Cs (orange) at several temperatures. Crosses stand for experimental data.

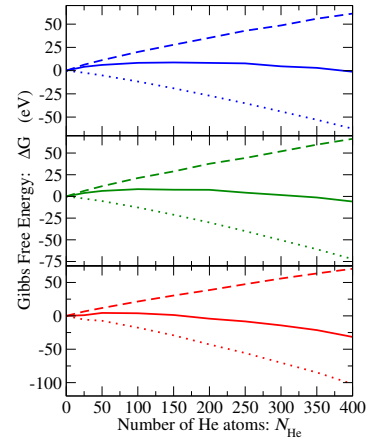


Fig. 2. Gibbs free energy of the He bubbles at temperatures of 470 K (blue), 657 K (green) and 843 K (red).

- [1] M. Korda and L. Koek, *Fusion Engineering and Design* **124**, 700 (2017).
- [2] M. Rubel, *Journal of Fusion Energy* **38**, 315 (2019).
- [3] H. U. Borgstedt, C. Guminski, H. U. Borgstedt, and C. Guminski, *Journal of Physical and Chemical Reference Data* **30**, 835 (2001).
- [4] D. Belashchenko, *Inorganic Materials* **48**, 79 (2012).
- [5] X. Sheng and K. Tang, *Physical Chemistry Chemical Physics* **23**, 7748 (2021).
- [6] L. Li, T. Totton, D. Frenkel, *The Journal of chemical physics* **146**, 214110 (2017).
- [7] S. Thompson, K. Gubbins, J. Walton, R. Chantry, and J. Rowlinson, *The Journal of chemical physics* **81**, 530 (1984).