

MD of liquid Lithium sputtering by He⁺ ions and bubble formation

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Outline

- **MD study of diffusion in He atom in liquid Li surface**
- **MD study of the Li sputtering Yields and He reflection coefficients for He⁺ ion collisions with a liquid He/Li surface**
- **He Bubble formation in liquid Li – MD, MC studies, review of the existing problems and outline of the future work**



Molecular Dynamics method

MD numerically calculates the classical equations of motion (EOM) on a computer i.e. it gives the phase space trajectories of a system.

$$\bar{A} = \lim_{t' \rightarrow \infty} \frac{1}{(t' - t_0)} \int_{t_0}^{t'} A(\mathbf{r}^N(t), \mathbf{p}^N(t); V(t)) dt,$$
$$\bar{A} = \langle A \rangle_{NVE}.$$

The physical variables could be obtained by averaging over the trajectories. E.g., T and P are calculated as follows:

$$T = \langle \mathbf{T} \rangle, \text{ where } \mathbf{T} = \frac{2}{3k_B T} \sum_{i=1}^N \frac{mv_i^2}{2}$$

$$P = \langle \mathbf{P} \rangle - \frac{\rho^2}{6} \int_{r_{cut}}^{\infty} r \frac{\partial \phi}{\partial r} g(\vec{r}) d\vec{r}, \quad \mathbf{P} = \rho k_B T - \frac{\rho}{3N} \sum_i \sum_{j>i} r_{ij} \frac{\partial \phi(r_{ij})}{\partial r_{ij}}$$

Here, $\phi(r_{ij})$ is the inter-particle potential function, ρ is the average density, $g(\vec{r})$ – the pair-correlation function – the probability for two particles to be a distance r .

Comparison with experiment

The MD diffusion coefficients are compared with experiments.

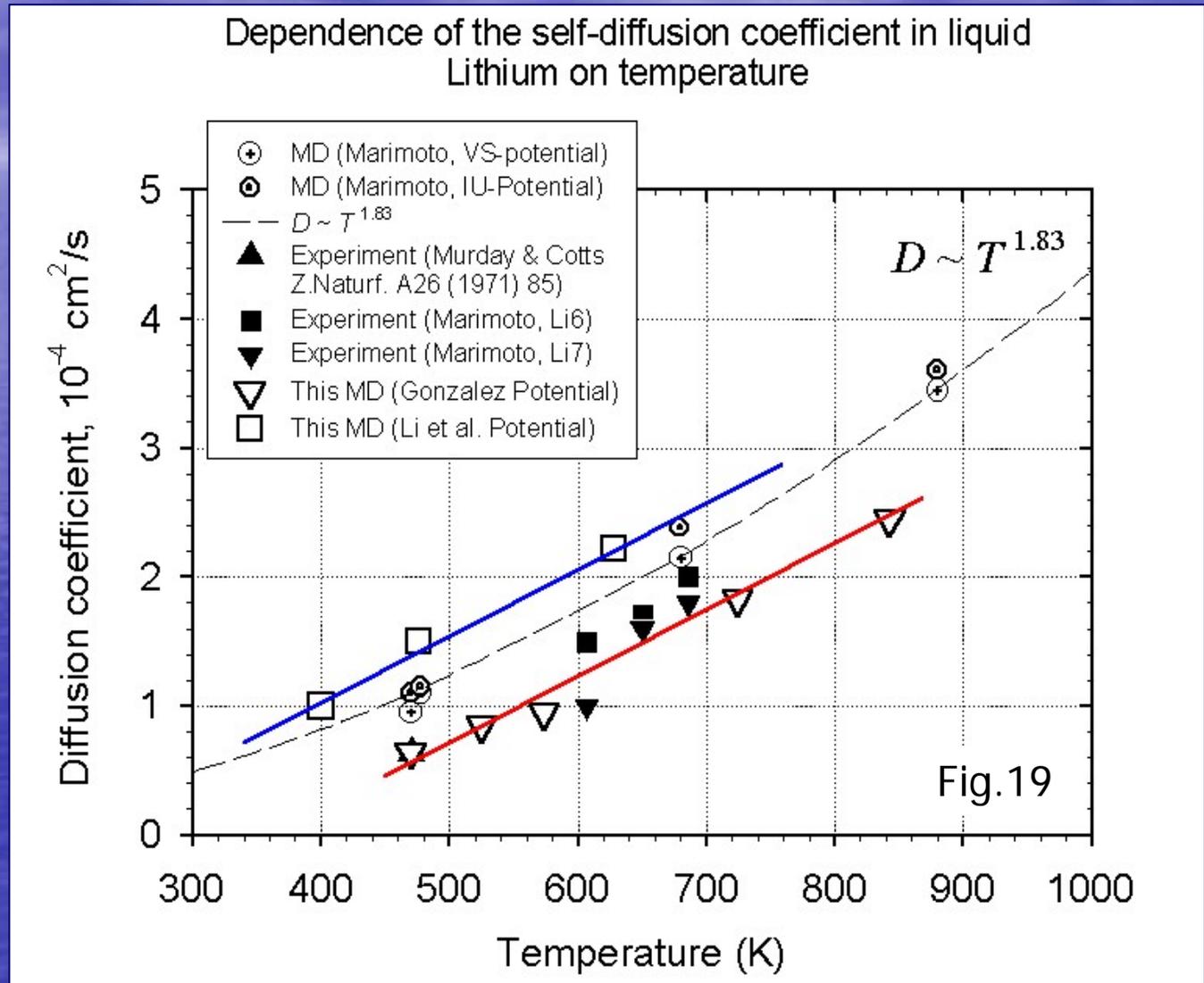
The red line is drawn as “an eye guide” for potential [1].

The blue line – for the potential [2] (Li et al.).

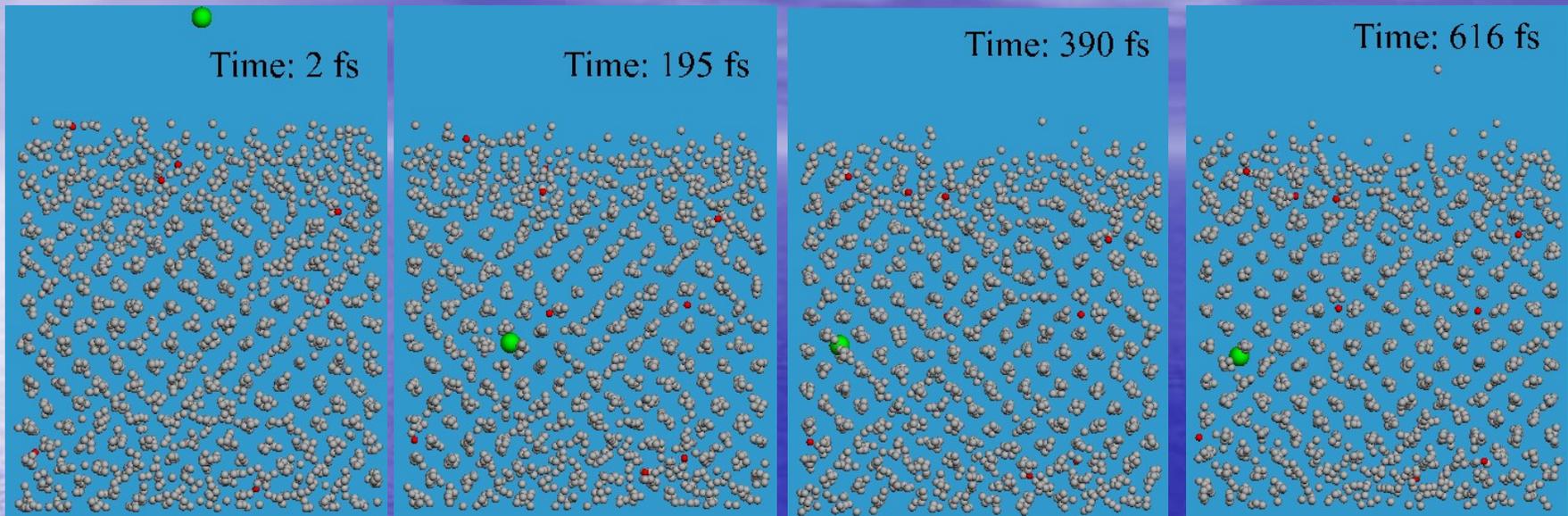
References:

[1]. M. Canales et al, Phys. Rev.E50 (1994) p.3656.

[2]. Y. Li et al, Phys. Rev. B57 (1998) p.15519.



He/Li sputtering with He⁺ ions



Comments for pure and He-saturated Li @ 470K:

- He⁺ ranges **may** decrease with the He content in Li – **this needs more analysis**;
- The analysis shows **more intense energy exchange** for the He saturated Li near the surface – **needs bigger system**;
- The Li sputtering Yield **could** increase with He content – **need more analysis**;
- Simulations are going on at higher temperatures for comparison

He bubbles in liquid Lithium

Motivation

The mechanisms of bubble formation in liquid metals are not well understood. They are important for liquid surface erosion under irradiation with He ions. There is a fundamental interest to this process [1].

Two processes, with different time scales:

1. Slow process – formation of a critical nucleus

MD will be used to calculate the binding energies and the kinetic coefficients. **This is a huge simulation task and will be performed in the future.** If the energies and kinetic coefficients are known, the rate equations or thermodynamic Saha equations solve the problem.

2. Fast process – Bubble collapse and sputtering

MD & MC simulations will be performed for collapse of a He bubble in liquid Li. PBC and a realistic Li-Li and He-Li potentials were used.



Kinetics of He Bubble formation in liquid

Kinetics of bubble formation

The kinetics of bubble (cluster) formation effects is a long studied subject in various areas. The Mean-field rate equations offer a complete obtaining concentrations of the bubbles (clusters).

$$\begin{cases} \dot{n}_1 = \Phi(z, t) - 2D\sigma_1 n_1^2 - 2D \sum_{s>1} \sigma_s n_1^2, \\ \dot{n}_s = Dn_1 \sum_{s>1} (\sigma_{s-1} n_{s-1} - \sigma_s n_s) - n_s \exp(-E_s / kT) \end{cases}$$

n_1 – the density of He atoms,

n_s – the density of bubbles with s ($s \gg 1$) atoms,

$\Phi(z, t)$ – Helium flux from plasma,

D – Helium diffusion coefficient,

σ_s – capture probabilities,

E_s – binding energy of a bubble

with s atoms.

Pro of the method

1) All kinetic parameters: diffusion constants, capture numbers, evaporation rates could easily be obtained from MD and this would give the complete solution of the problem.

Contras of the method

1) Only monomers are mobile – which is not true as dimers and other polymers are also mobile. This increases the number of equations and needs the diffusion coefficients of big He-clusters.

2) The capture coefficients are far below unit – our MD simulations show that.

3) Evaporation of clusters occur not only by single atoms, but by dimers, trimers, etc.

4) The rate equations belong to a class that is called "stiff" – the different cluster sizes have widely different time scales.



Summary

- Our **MD** simulations of liquid Lithium show that **MD** has great capabilities for calculations of diffusion constants. Indeed, **MD can do much more: it could be used to study near the surface processes for liquid metals.** However, we need good potentials.
- Preliminary MD calculations of He/Li sputtering Yield bombarded with He⁺-ions with $E < 100\text{eV}$ have been carried out for liquid Li and they show that **MD** is a straightforward computational PMI method, without any adjusting parameters.
- **MD & MC** methods has been used to study the kinetics of small He bubble formation. **MD** could be used to finding the rate coefficients and the binding energies of the small bubbles.
- Future study should be concentrated on the rate and Saha equation approaches -- **a huge computational task of computing the kinetic coefficients and formation energies for the new phase.**

