Contribution ID: **21** Type: **Talk**

Machine-learning interatomic potential development for an atomistic study of tritium diffusion in liquid lithium and lithium-vanadium interfaces

Thursday 5 February 2026 11:35 (30 minutes)

Liquid lithium is a candidate material for tritium breeding and as a coolant in fusion reactors. Vanadium is proposed as the corresponding structural material surrounding the liquid lithium, owing to their compatibility. However, tritium retention and transport in liquid lithium and across a lithium-vanadium interface is either ambiguous or unknown from literature, which prevents an accurate modelling of the tritium inventory. Atomistic simulation techniques such as molecular dynamics (MD) provide a way to understand the mechanism and calculate relevant properties. The accuracy of the results relies on the interatomic model used for the system. In the first part of this work, we show MD simulations of hydrogen isotope diffusion in liquid lithium using a newly developed atomic cluster expansion (ACE) machine-learning interatomic potential (MLIP) [1]. We resolve long-standing deviations in experimental data of diffusivities (shown in Fig. 1), and analyze the diffusion mechanism in the liquid metal. In the second part, we discuss the development of two comparable MLIPs –the ACE and a neuroevolution potential (NEP) [2] –to study the lithium-vanadium-tritium system. Specifically, we calculate the solution energies of tritium at different interfaces and the temperature-dependent transport of tritium across the interface. The results from MD simulations will be useful for parameterizing and formalizing gas transport equations in future.
Acknowledgements: The project is funded through the LIBRTI programme at the UKAEA.
[1] P. Srinivasan, S. Puri, K. Pacho Dominguez, A.P. Horsfield, M.R. Gilbert and D. Nguyen-Manh, Atomic cluster expansion interatomic potentials for lithium: investigating the solid and liquid phases, Physical Review B 112, 054108 (2025) https://doi.org/10.1103/q4nm-qyk4
[2] Z. Fan, Z. Zheng, C. Zhang, Y. Wang, K. Song, H. Dong, Y. Chen and T. Ala-Nissila, Neuroevolution machine learning potentials: Combining high accuracy and low cost in atomistic simulations and application to heat transport, Physical Review B 104, 104309 (2021) https://doi.org/10.1103/PhysRevB.104.104309
[3] H. Moriyama, K. Iwasaki and Y. Ito, Transport of tritium in liquid lithium, Journal of Nuclear Materials 191-194, 190-193 (1992) https://doi.org/10.1016/S0022-3115(09)80031-7
[4] S. Fukada, M. Kinoshita, K. Kuroki and T. Muroga, Hydrogen diffusion in liquid lithium from 500 ℃ to 650 ℃, Journal of Nuclear Materials 346, 293-297 (2005) https://doi.org/10.1016/j.jnucmat.2005.06.021

Speaker affiliation

UK Atomic Energy Authority

Author: SRINIVASAN, Prashanth (United Kingdom Atomic Energy Authority)

Co-authors: Ms COLLINS, Rebecca (University of Southampton); Mr PITIKE, Krishna Chaitanya (Pacific Northwest National Laboratory, USA); Mr SETYAWAN, Wahyu (Pacific Northwest National Laboratory, USA); GILBERT, Mark (UKAEA); Mr NGUYEN-MANH, Duc (United Kingdom Atomic Energy Authority)

Presenter: SRINIVASAN, Prashanth (United Kingdom Atomic Energy Authority)

Session Classification: Session 3-10

Track Classification: LIBRTI Conference