Thermodynamic Integration Calculations for Helium Solubility in Lead-Lithium Alloys

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Lead-lithium stands out as a liquid metal breeder in many current nuclear fusion reactor designs. During the production of tritium in the breeding blankets helium outcomes as a by-product. The noble gas is known to have a very low solubility in many liquid metals, such as lithium itself. No experimental measurements have been made, up to date, to determine the solubility of helium in pure lead or in lead-lithium melts. As far as we get from the solubility threshold, it is more possible for helium to nucleate inside the reactors. The lead-lithium eutectic composition (15.7-17% at. % Li) is of particular interest, since it is often proposed as a breeding material. We use the thermodynamic integration scheme to characterize LLE and helium solubility from molecular dynamics simulations.

As a previous step to the inclusion of helium, the properties of lead-lithium melts predicted by our model have been compared with experimental data. In particular, free energy methods are used to reproduce the phase diagram around the eutectic point.

Henry's law says that the fraction of gas dissolved in a liquid solvent is proportional to the pressure that this gas exerts on the liquid. Henry's constants of helium in liquid lead-lithium alloys are calculated from free energy methods based on thermodynamic integration.

In the calculations, we explore a region of the phase diagram around the predicted eutectic point of the lead-lithium system, from the eutectic temperature (508 K) up to high temperatures (~1000 K). We study the dependence of Henry's constants on both the temperature and solvent composition.

Finally, in order to describe the onset of nucleation, free energy barriers are estimated from the computed Henry's constants.