Nucleation of helium in molten lithium

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In the breeding blankets of nuclear fusion reactors tritium and helium (He) are produced in the same amount (mol-to-mol) from neutron capture reactions by lithium (Li) isotopes. The resulting He, which has a very low solubility in liquid metals (LM), may nucleate affecting the behavior of the BB (magneto-hydrodynamic flow and transport properties, electrical conductivity, etc.). Due to safety reasons, liquid lead-lithium (LiPb) eutectic alloy is preferred over pure Li as the breeding material. The molecular dynamics method is implemented, using both LAMMPS package [1] and Fortran codes, to simulate the phenomenon of He nucleation in pure molten Li as a first step to characterize its behavior in LiPb alloys. The most fundamental step to understand and describe our systems is finding the best choice of interatomic potentials. Starting from pure Lennard-Jones (LJ) interactions and other simple models [2-4], which reproduce the segregation of Li and He phases quite well (see, for instance, figure 1), but overestimate the Li-He repulsion, we have moved to more refined models: figure 2 shows the Toennies-Tang-Sheng (TTS) potentials [5,6] for He-He and Li-He, which have a softer repulsive region compared to the steep wall of LJ potentials but similar wells (both position and depth), while figure 3 presents both embedding function (electronic density contribution) and pair potential of Embedded Atom Models (EAM) [6-9] for the LM. We rely on the accuracy of radial distribution functions and thermo-physical properties (such as density and diffusion coefficients), compared to experimental data, to validate the chosen set of interatomic potentials. Other issues related to the potentials, such as the computational complexity, have also been considered. In addition, other properties such as surface tension of He bubbles have been studied. The onset of nucleation is studied by means of the Henry's constant. We explore moderate thermodynamic states in which temperature is below the boiling and above the melting points of both pure molten Li and LiPb eutectic and ambient-like pressures (typically of 843 K and 1 bar).

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FIGURES

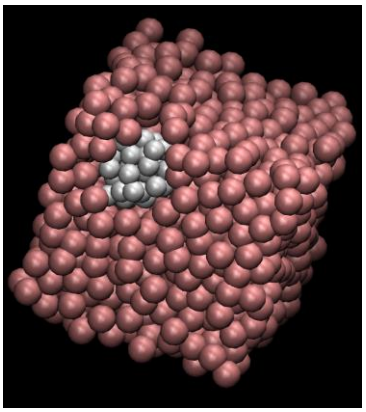

Figure 1: Snapshot of a cluster of 40 He atoms in a simulation box with 1000 Li.

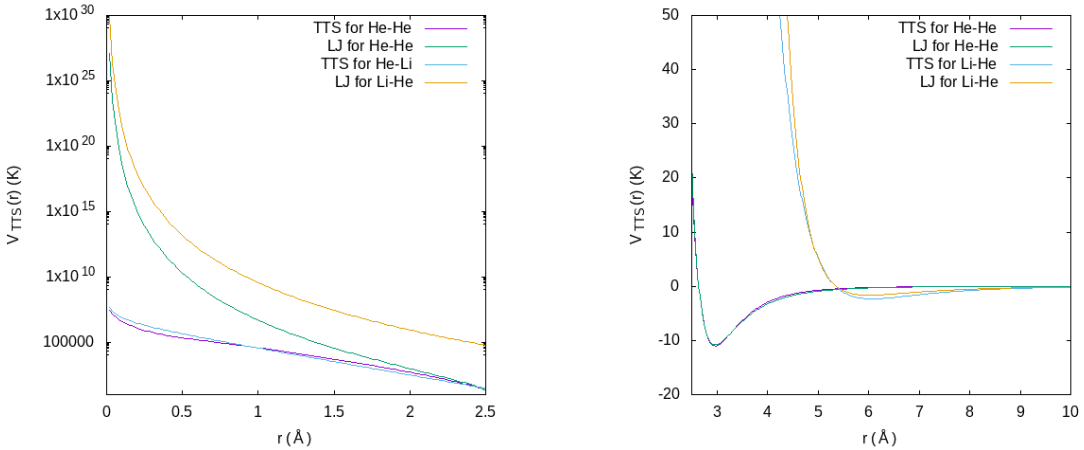

Figure 2: Comparison of LJ and TTS potentials for pair (helium-helium and helium-lithium) interactions. Both short (left, logarithmic scale for the y-axis) and long (right) ranges are represented.

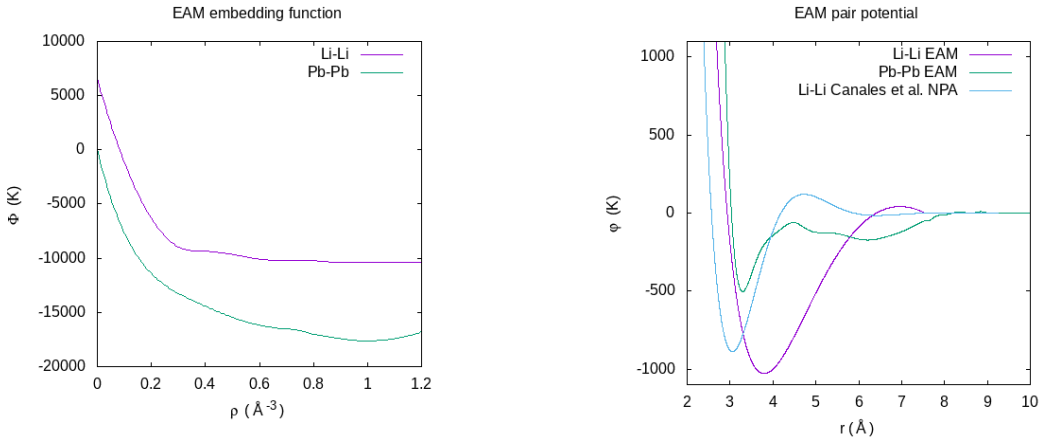

Figure 3: Embedding function and pair contribution of lithium-lithium and lead-lead (EAM) potentials.