Liquid lithium and lead: A comprehensive molecular dynamics study.

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1. INTRODUCTION

- Pb17Li is today a reference breeder material in diverse fusion R&D programs worldwide. One of the main issues in these programs is the problem of liquid metals breeder blanket behavior. Structural material of the blanket should meet high requirements because of extreme operating conditions. Therefore the knowledge of eutectic properties like optimal composition, physical and thermodynamic behavior or diffusion coefficients of Tritium are extremely necessary for current designs. In particular, the knowledge of the function linking the tritium concentration dissolved in liquid materials with the tritium partial pressure at a liquid/gas interface in equilibrium, $C_T=f(P_T)$, is of basic importance because it directly impacts all functional properties of a blanket determining: tritium inventory, tritium permeation rate and tritium extraction efficiency. Nowadays, understanding the structure and behavior of this compound is a real goal in fusion engineering and materials science. Simulations of liquids can provide much information to the community; not only supplementing experimental data, but providing new tests of theories and ideas, making specific predictions that require experimental tests, and ultimately helping to lead to the deeper understanding and better predictive behavior.

2. LITHIUM AND LEAD MD SIMULATIONS

- We have implemented several EAM potentials both for Pb [1] and Li [2] to carry out Classical MD simulations (LAMMPS) as previous step to develop a Pb-Li cross-potential.

$$E_i = \sum_j \phi(r_{ij}) + F\sum_j \rho(r_{ij})$$

φ is a pair-potential interaction between atoms i and j and F is an embedding function, (the energy to embed atom i in the electron density ρ provided by its surrounding j atoms).
The φ, ρ, and F functions are analytic expressions with coefficients fited to various experimentally determined quantities.

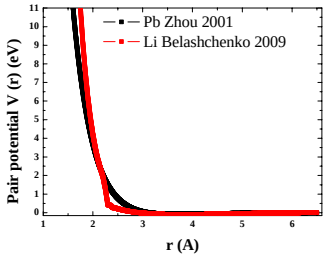


Figure 2.1: EAM pair potentials for pure elements Pb and Li.

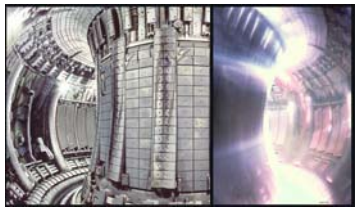


Figure 2.2: JET chamber.

Not only LiPb will be important for future nuclear fusion reactors. For example, liquid lithium is a very promissing candidate for plasma protecting components and divertor technologies..

- Information obtained from these calculations will be properly processed and used as input for classical MD codes in order to evaluate kinetics and diffusion phenomena in the eutectic.
- In the near future the interaction of Pb17Li with single species like tritium and/or helium will be carefully modeled in the context of breeding blanket modules.
- This is of scientific and technological importance because physical properties like solubility of He and T in liquid metals are difficult to measure.

3. MD SIMULATIONS VS EXPERIMENTAL RESULTS

- Liquid Li and Pb has been simulated with the mentioned EAM potentials [1] [2]. Both potentials give good agreement with experimental values. Here we show some static, structural and thermodynamic properties calculated from our MD simulations compared with experimetal data.

	Experimental		MD	
	ρ (Liq Tem) g/cm³	∂ρ/ ∂T (g/cm³K)	ρ (Liq Tem) g/cm³	∂ρ/ ∂T (g/cm³K)
Li	0,51	-9,6x10^{-5}	0,53	-8,6x10^{-5}
Pb	10,64	-0,0013	10,96	-0.0013

3.1 Radial Distribution Functions

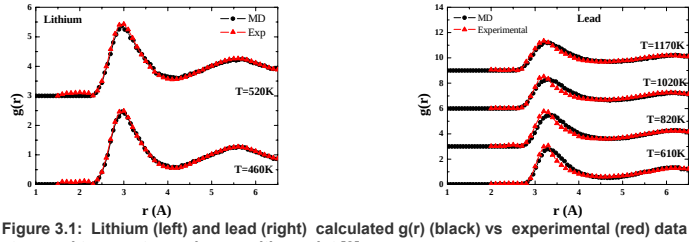


Figure 3.1: Lithium (left) and lead (right) calculated g(r) (black) vs experimental (red) data at several temperatures above melting point [3].

3.2 Heat Capacity and Density

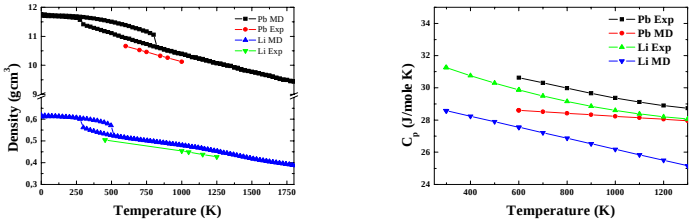


Figure 3.2: Calculated Li and Pb densities (left) and heat capacities (right) compared with experimental data.

4. MELTING POINT

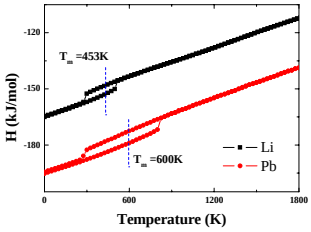


Fig 4.1. Calculated enthalpy for pure Pb and Li. Blue dashed line signals the experimental melting point.

Free energies can be calculated using the Gibbs-Duhem integral [4]:

$$F(T) = f(T_0)\frac{T}{T_0} - T\int_{T_0}^{T}\frac{h(\tau)}{\tau^2}d\tau$$

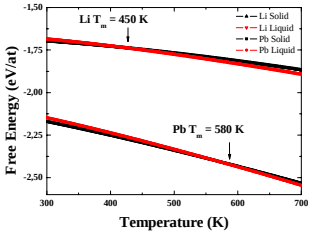
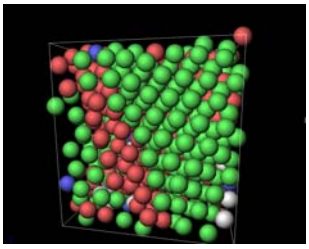


Fig. 4.2. Free energies of solid (black) and liquid (red) Pb and Li calculated with the thermo-dynamic package using the EAM potentials described above. The calculated melting points for Pb and Li are respectively 580K and 450K, the experimental values are 600 and 450 respectively.

5. PRESSURE



Experimentally, lithium presents a structural phase transition (from bcc to fcc lattice) at high pressures [5], exactly at 7.5 GPa. Lithium potential seems good enough to acount on that transformation.

Figure 5.1 Lithium CNA analysis visualization at 2000 K and P= 8Gpa. (N=686 Atoms). Green spheres correspond to fcc atoms, red ones to hcp, blue to bcc and white to others.

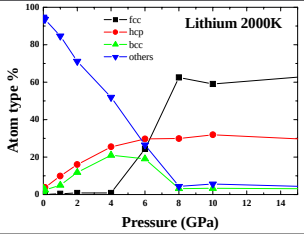


Figure 5.2. Lithium CNA analysis at 2000K at different presures (N=686 Atoms). Some ordering to a fcc structure takes place around 7 GPa, as expected.

Similarly, lead presents a structural phase transition (from fcc to hcp lattice) at high pressures [6].

6. CONCLUSIONS

- Physical properties of lithium-lead eutectic alloy should be determined carefully in order to study the suitability of the alloy for blanket modules.
- We have implemented EAM potentials for Li and Pb metals in LAMMPS scripts. Both potentials give reliable results in the liquid phase.
- We have implemented a new LiPb EAM/cd cross potential [7].
- The results obtained from QMD and/or CMD will be very helpful in order to complete the experimental database.
- Intense magnetic field (up to 5T) effects in physical properties of the alloy must be studied.
- The behaviour of tritium and helium inside the liquid metal is still far from being understood. Molecular dynamics simulations are paramount to understand and analyze current experiments.

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