New simulations to qualify eutectic lithium-lead as a breeder material

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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 is the problem of liquid metals breeder blanket behavior. 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. Atomistic simulations of liquids can provide much information; not only supplementing experimental data, but providing new tests of theories and ideas, making specific predictions that require experimental tests, and ultimately helping to a deeper understanding.

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 alloy 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.

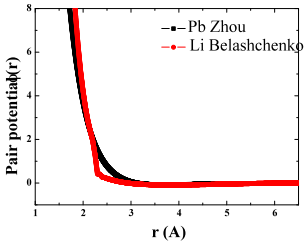


Figure 2.1: EAM pair potentials for pure elements Pb [1] and Li [2].

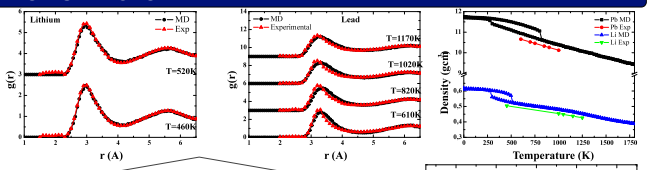


Figure 2.2: Lithium (left) and lead (center) calculated g(r) vs experimental data above melting point. Right) Density vs T.

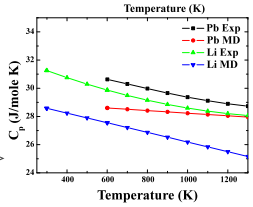


Figure 2.3: Calculated Li and Pb heat capacities (right) compared with experimental data.

3. Li-Pb EAM/CD ALLOY POTENTIAL

An EAM composition dependent (EAM/cd) alloy potential [3] has been developed. In this formalism the alloy potential is multiplied by a grade four polynomial in composition used as adjustable parameter to fit the enthalpy of mixing.

3.1 Heat of mixing

In order to create a LiPb potential valid for all the Li concentration range we used as target the experimental heat of mixing at 800 K and 1000 K.

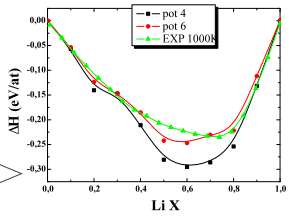


Figure 3.1: Calculated heat of mixing at 1000 K with 2 different potentials compared with experimental data (green triangles).

3.2 Eutectic simulation

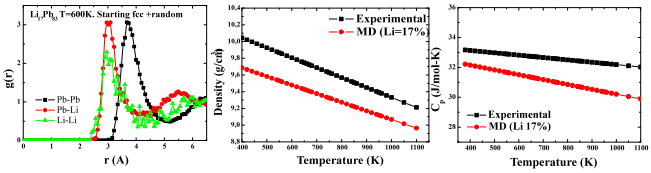
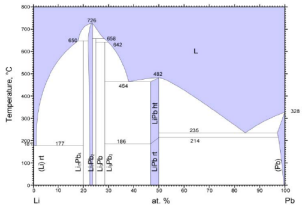


Figure 3.2. (Left) Calculated partial g(r)s of Li17Pb at 600K (experimental data in table below [6]), (centre) density vs Temperature and (right) heat capacity, C_p, compared with experimental data [4].

T(K)	g_{ij}(r)	Exp r_1	MD r_1	g_{ij}(r)	Exp r_1	MD r_1	g_{ij}(r)	Exp r_1	MD r_1
508	**Pb-Pb**	3.55	3.73	**Pb-Li**	2.79	3.02	**Li-Li**	2.40	3.05
593		3.54	3.67		2.77	2.95		2.76	2.9

4. CRITICAL PHYSICO-CHEMICAL PROBLEMS

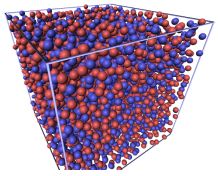
4.1 PHASE DIAGRAM



First input in the experimental database that must be clarified is the exact proportion of Li and Pb in order to have a true eutectic alloy [5].

A theoretical determination of the Li-Pb phase diagram is in progress [6].

4.2 LIQUID STRUCTURE



Experimentally, liquid $Pb_{17}Li$ seems to consist in Li_4Pb complexes and Pb_n clusters [7].

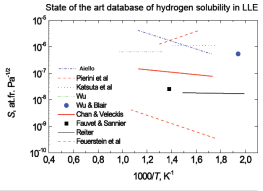
The survival of Li_4Pb ions in the liquid phase could be technologically important. The magnetic properties and the effect of the intense magnetic fields in the liquid melt will be carefully studied.

Figure 4.1. Snapshot after a MD heating run up to 1300K of a Li50Pb50 sample starting from a fcc lattice (N=10000).

4.3 HELIUM AND TRITIUM

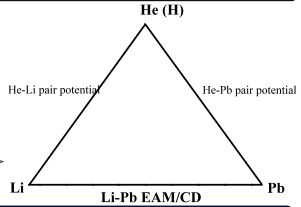
The extraction rate of tritium from LiPb has been studied as a function of T. However there is no data on the effect of the bubble diameters on the extraction rate, key factor to design the tritium extraction system.

Tritium solubility database is inadequate for design. Knowledge of dynamic transport properties (diffusion, mass transfer, interface processes) is much more limited [8].



4.4 FUTURE PLANS

He(T)-Pb and He(T)-Li potentials are being developed.
He (and/or T) will be introduced in LiPb simulations.



Schematic picture of the ternary potential for Li-Pb-He.

5. CONCLUSIONS

We have implemented EAM potentials for Li and Pb metals in LAMMPS scripts and developed a new Li-Pb EAM/cd alloy potential.

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 [8].

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REFERENCES

[1] Zhou *et al* Acta Materialia Vol 49, Issue 19, 14 November 2001, 4005-4015

[2] D. Belashchenko *et al.* High Temperature 2009 vol 47 No 2 211-218.

[3] A.Caro, D. A. Crowson, and M. Caro. PRL 95, 075702 (2005)

[4] M. Vals *et al*, Journal of Nuclear Materials 376 (2008) 353-357

[5] P. Hubberstey, T. Sample and M. G. Barker, J. Nucl, Mater 191-194, 283-287 (1992)

[6] A. Fraile, A. Caro, S. Cuesta *et al.* In progress.

[7] S. Mudry *et al*, Journal of Nuclear Materials 376 (2008) 371–374

[8] LIBRETTO. N. Moral *et al.* In progress