MD MULTISCALE STUDIES SUPPORTING LITHIUM-LEAD EUTECTIC ALLOY DATABASE

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Lead-lithium eutectic (LLE) is a well-consolidated candidate as tritium breeding functional material. LLE material´s database is today under construction having quality assurance requirements of a nuclear material. Most part of the LLE database is constituted by experimental entries but LLE key material´s database can be supported and extended by the use of MultiScale Modelling (MsM) computational approaches. Some of the needed database entries can be obtained with severe experimental difficulties or uncertainties and MsM offers an alternative way to obtain them. Computational algorithms in classical Molecular Dynamics are well established to derive any LLE material property of interest of fusion nuclear technology as: theoretical Li-title of the ideal eutectic composition, density, dynamic viscosity, surface tension, tritium or helium gas solubility and many others. Liquids are, in this sense, more simple than solids to simulate their properties.

Firsts steps of MsM work focus on LLE binary alloy structural information, e.g.: constituents pair correlation function *g(r)* or *Structure´s factor* S(k). Unfortunately, neutron diffraction data is not available today for LLE to validate Structure factor predictions by MSM of LLE.

Today there is not a validated Li-Pb pair potential capable to predict LLE properties and for the moment the work should follow a procedure consisting in the validation of potentials through the alloying mono components: Pb and Li themselves. This line is pursued at present by implementing several potentials (EAM, MEAM, FS, etc) both for Pb and Li to carry out classical MD simulations using LAMMPS and reproducing their properties as mono-constituents. Capabilities to reproduce database are shown.

Thus, for the jump into binary LLE quantum ab initio calculations are needed in order to develop a suitable Li-Pb potential. This R&D way is being explored.

Some preliminary assessments of Li-Pb potential characteristics are reported.

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