Molecular Dynamics simulation of liquid metals for nuclear fusion technology

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Abstract

Liquid metals and alloys could be present in future nuclear reactors as breeder blankets (coolant and tritium production system) and/or plasma facing materials in wet walls, divertors in magnetic confinement reactors etc [1, 2]. In breeding blankets tritium and helium will be produced by Li splitting but tritium extraction and tritium interaction with helium bubbles is still far from being well understood. Lithium-Lead eutectic alloy is one of the most promising candidates because of its low chemical activity compared to pure lithium and good breeding ratio [3]. Here we present some atomistic simulations in hydrogen liquid metal systems. We have studied H (and its isotopes) diffusion in two different liquid metals making use of two different interatomic potentials, namely an Embedded Atom Method (EAM) potential for Pd-H system [4] and one more advanced EAM/angular dependent potential for Al-H system [5]. A full theory of H behavior in liquid metals is, to date, lacking and experimental results are scarce. Also we have developed a Li-Pb EAM interatomic potential capable to predict LiPb eutectic properties [6] after careful validation of Li and Pb EAM potentials [7-9]. Capabilities to reproduce database are shown. We address several features dealing to H diffusion in liquid metals as well as self diffusion of Li in LiPb systems.

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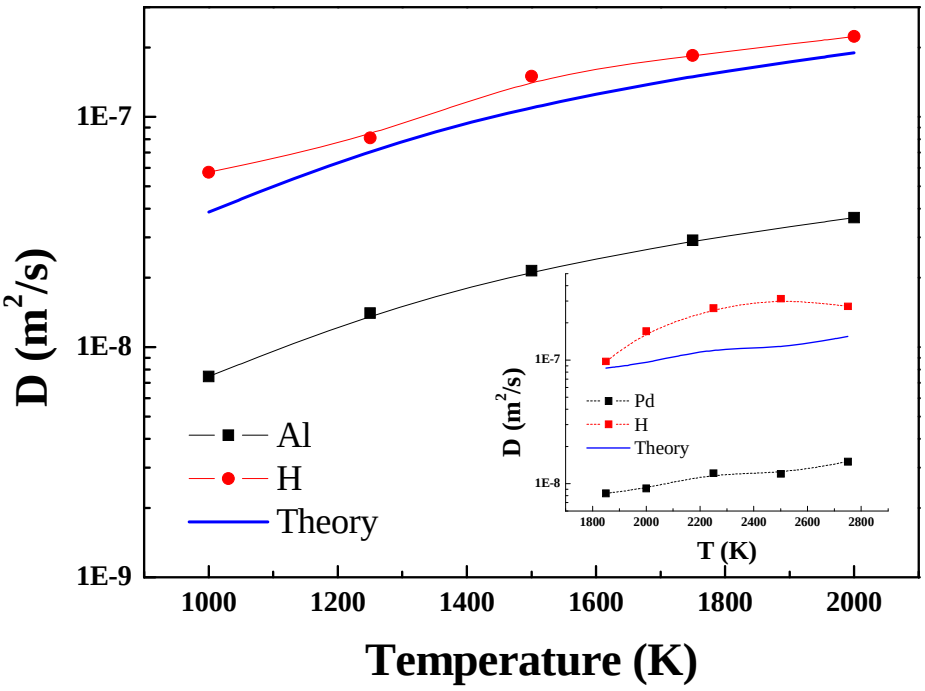

Figure 1. Diffusivity values for H in Al and Pd (see inset) compared with host metal self-diffusivity (black squares). H diffusivity (blue line) is close to the calculated (red = Theory) just as $D_H = D_M\sqrt{m_M}$ where m_M stands for the mass of the host metal.