PLASMA-MATERIAL INTERACTION IN FUSION DEVICES

Dissolution corrosion and embrittlement of iron in liquid lead-lithium alloys

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Introduction

The liquid metal lithium-lead blanket design is one of the most promising designs for future fusion power plants [1]. The corrosion of structural steel in liquid lithium-lead eutectic becomes the restraining factor for fusion reactor design and secure operation [2-4]. Using the first-principles calculations, we'll investigate the effects of liquid metal on iron by exploring behaviors of liquid metals on surfaces and at grain boundaries. The dissolution corrosion can be determined by calculating adsorption energies of metal atoms in liquid phase and escape energies of surface Fe atoms. Besides, the embrittlement can be characterized by strengthening energies and separation energies. Finally, the corrosion origin will be also derived by electronic charge analysis. This work will be helpful for evaluating the dissolution corrosion and embrittlement capabilities of liquid lead-lithium and selecting alloys with good corrosion resistance.

Methodology and models

The simulations in this work were performed using density functional theory as implemented in the Vienna *Ab-initio Simulation Package* (VASP). The projector augment approximation wave potentials (PAW) and the generalized gradient approximation (GGA) with the exchange-correction functional proposed by Perdew-Burke-Ernzerhof were employed in the calculations. The wave functions were expanded in the plane-wave basis set using an energy cutoff of 400 eV. The Fe(100) surface and grain boundaries of Σ3(111) and Σ5(310) were constructed to explore the corrosion and embrittlement of Li towards steels. The Brillouin zone integrations were performed on a special k-points mesh, 5×5 × 1 for the Fe(100) and 15 × 5 × 1 for the grain boundaries, generated by the Monkhorst–Pack scheme.

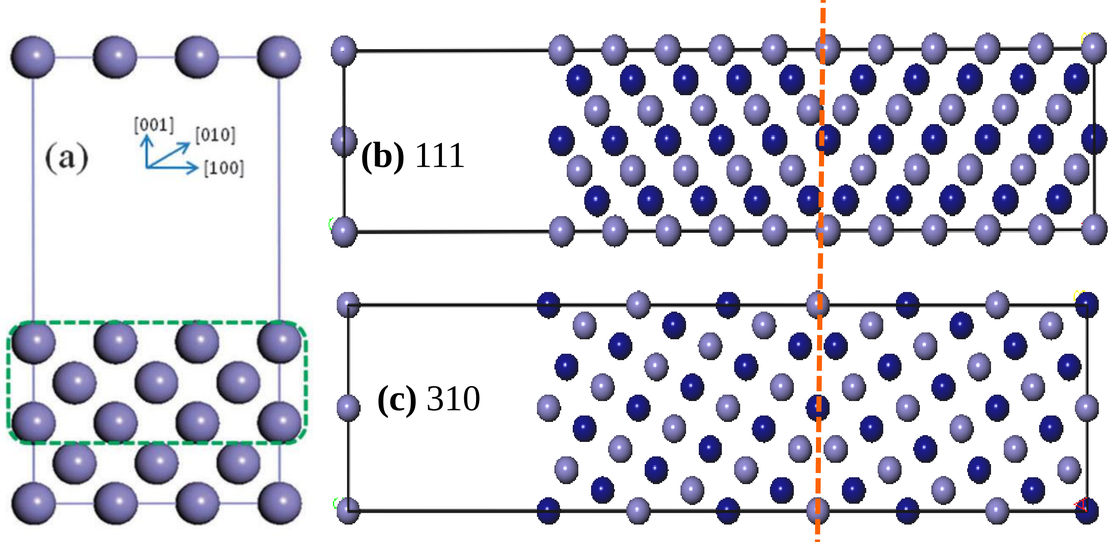

Fig.1 The Fe-slab with (001) surface on (a), grain boundaries of Σ3(111) and Σ5(310) on (b) and (c), respectively. The grain boundaries are labeled by the red line.

Conclusions

The corrosion and embrittlement of Li and Pb have been investigated by theoretical calculations based on the density functional theory (DFT). Li and Pb atoms on the Fe(100) surface promote dissolution corrosion, which decreases with increase of coverage. Meanwhile, Li and Pb at Fe grain boundaries also accelerate embrittlement of Fe-based materials. Both the corrosion and embrittlement of Li atoms are caused by the significant charge transfer between Fe atoms and impurities.

References

1. V. Tsisar *et al.*, Corros. Sci. 53 (2011) 441–447.
2. Xizhang Chen *et al.*, Corrosion Science 96 (2015) 178–185.
3. N. Simon *et al.*, Corros. Sci. 43 (2001) 1041–1052.
4. G. Benamati *et al.*, J. Nucl. Mater. 307 (2002) 1391–1395.

Results

1. *Corrosion of Li on the Fe(100) surface*

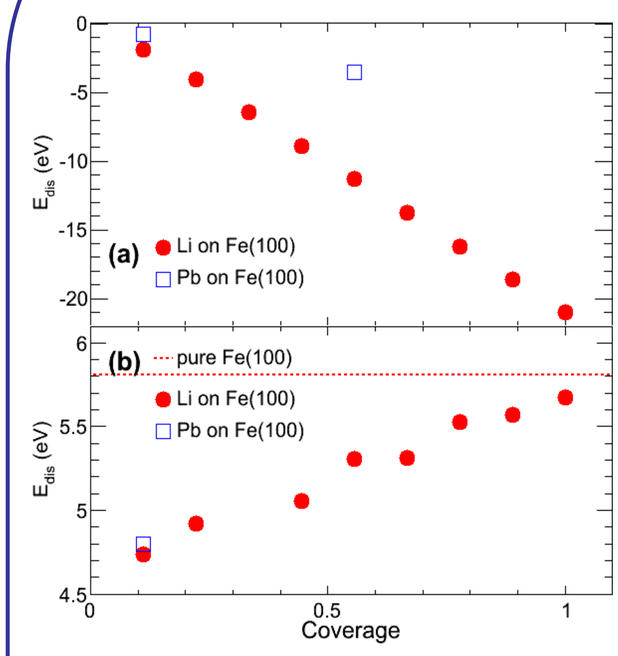

Fig.2 Adsorption energies of Li and Pb on the Fe(100) surface (a) and dissolution energies of Fe and Pb on the Fe(100) surface with Li adsorbed.

Li and Pb can be easily adsorbed on Fe(100) surface, and their adsorption energies decrease with the increase of their coverage. Besides, Li can be adsorbed more easily than Pb atoms. The dissolution capability of Li greater than that of Pb, is weaken with the increase of its coverage.

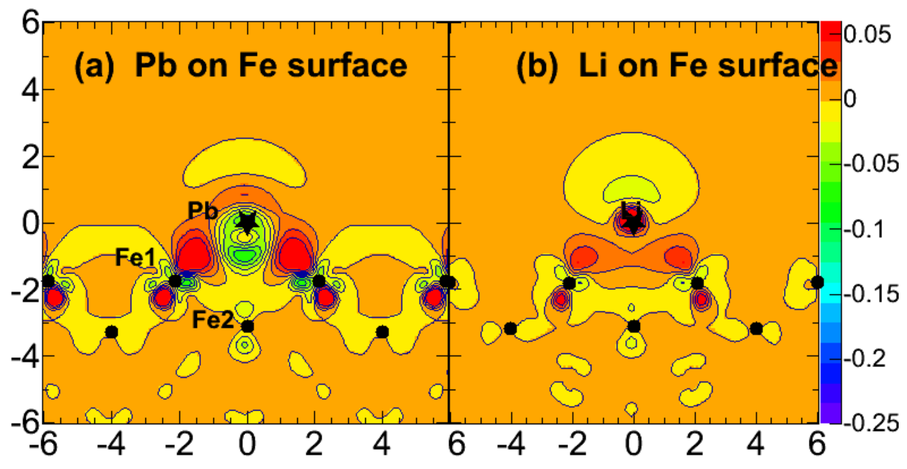

Fig.3 Charge density difference of Pb (a) and Li on the Fe(100) surface. The unit is electrons per Å^3.

Li and Pb can be adsorbed on Fe(100) surface easily at hollow position, thereby accelerating the dissolution of surface Fe atoms.

2. *Embrittlement of Li at Fe grain boundaries (GB)*

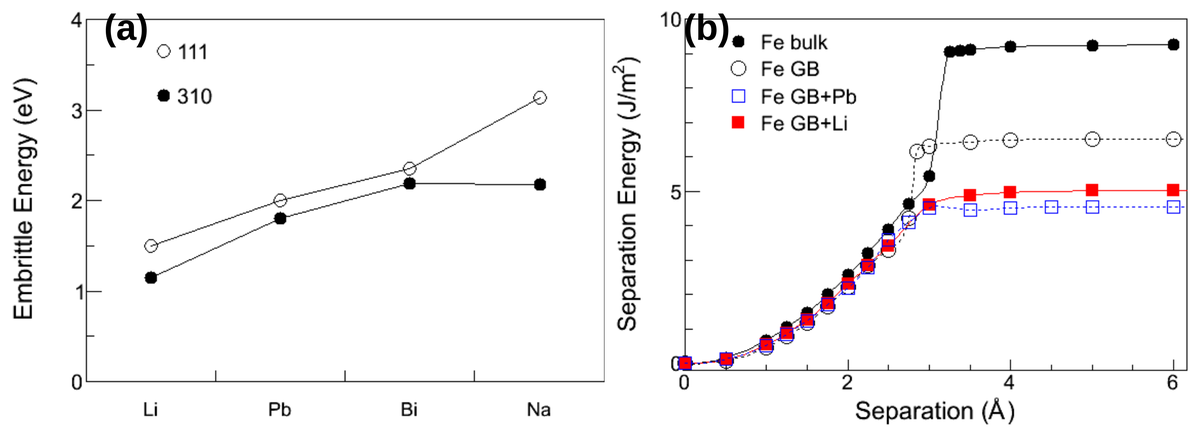

Fig.4 (a) Embrittlement energy of Σ3(111) and Σ5(310) GB with segregated Li, Pb, Bi and Na; (b) Separation energies of Fe bulk, pure Σ3(111) GB, and Separation energies of Σ3(111) GB with segregated Li and Pb.

Li segregated into grain boundaries promote the embrittlement of grain boundaries. The embrittlement of Li is weaker than other impurities (Pb, Bi and Na).

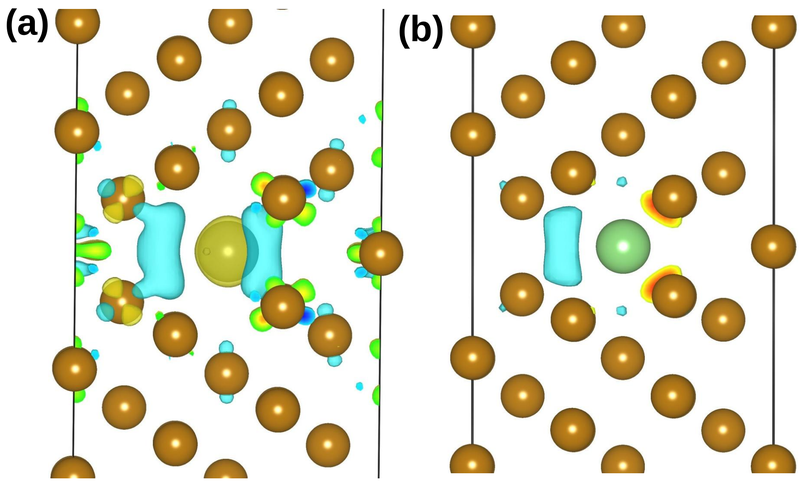

Fig.5 Charge density difference of Σ3(111) GB with segregated Pb (a) and Li (b). The isosurface of charge density is 0.034 e/Å^3. Blue region with negative values indicates a depletion of local electrons and yellow region (positive values) indicates an accumulation of local electrons.

Obvious charge transfers between impurities (Pb and Li) and Fe atoms around the grain boundaries, resulting in a depletion area between Fe atoms from different grains. This indicates Li and Pb can accelerate embrittlement of Fe GBs.