Insights into the initial corrosion stage of iron in liquid lead bismuth eutectic

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Abstract Excellent compatibility of the main candidate structural materials steels with the primary candidate coolant, liquid lead bismuth eutectic (LBE), poses great challenge to the deployment of lead-cooled fast reactors and accelerator-driven systems where LBE is used as the candidate primary coolant as well as spallation target [1]. Insights into the initial corrosion stage of steels in liquid LBE, which may significantly affect the later stage corrosion, are fundamental to figure out ways for surface treatment to improve their corrosion resistance. An Fe-Pb-Bi-O machine learning potential adopted molecular dynamics simulations [2] and first-principles calculations have been performed to explore the initial corrosion behaviors of bcc Fe surfaces exposed to liquid LBE. Both dissolution and oxidation are found to be dramatically dependent on the surface orientation, and the delicate balance between dissolution and oxidation leads to the observed corrosion anisotropy. In addition, effects of Cr addition on the oxidation and dissolution of bcc Fe surface have been also studied by first-principles calculations. A series of minutes level oxygen controlled experiments show that the initial oxidation process starts with oxygen adsorption followed by nucleation and growth of oxide films to different shapes, and this process is obviously inhibited by dissolution at either higher temperatures or lower oxygen content environments. Furthermore, both Fe_2O_3 and Fe_3O_4 are found on the corroded Fe surface even at low oxygen content in the early corrosion stage.

Keywords liquid LBE corrosion, computer simulation, oxidation, dissolution

Reference

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