5 - 11 Influence of Temperature on Early-stage Corrosion of bcc Fe Surfaces in Oxygen Dissolved Liquid Lead-bismuth Eutectic (LBE-O)

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The Lead-cooled Fast Reactor (LFR) is one of the fourth- generation nuclear energy systems with excellent development prospects. Liquid lead-bismuth eutectic (LBE) (44.5wt.% Pb + 55.5wt.%Bi) appears to be a promising candidate as a coolant for LFR due to its low melting point of 397 K, fast heat removing from the target, good neutron yield and low vapour pressure. However, the liquid LBE is corrosive to both austenitic steels and ferritic-martensitic steels, which are the main candidate structural materials for LFR. Therefore, corrosion considerations are essential in selecting appropriate structural materials and operating parameters in LFR. In general, dissolution/chemical reaction rates and corrosion product diffusion coefficients in solid and liquid alloys are functions of temperature. Therefore, it is important to investigate the temperature effect on early-stage corrosion of bcc Fe surfaces in oxygen dissolved liquid lead-bismuth eutectic (LBE-O). Molecular dynamics (MD) simulations on metal corrosion can provide a valuable complementary tool to investigate both the dissolution and oxidation characteristics of metals at the nanoscale[1,2]. We used a global neural network (G-NN) machine learning potential[3] molecular dynamics simulations to demonstrate the influence of temperature on the dissolution and oxidation behaviors of bcc Fe(100) surface contacting with oxygen dissolved liquid lead-bismuth eutectic.

As shown in Fig. 1, at about 550 ℃, the number of leaving-Fe atoms increases significantly. The number of leaving-Fe atoms is smaller than 5 when the temperature is below 550 ℃, while it is larger than 15 when the temperature reaches 550 ℃. The number of penetrated- Pb/Bi atoms is plotted in Fig. 1. It shows roughly the same trend as that of the number of leaving-Fe atoms. As shown in Fig. 2, when the temperature is between 470 and 500 ℃, the penetration depth of Pb/Bi atoms always fluctuates around a low value of about 0.5 Å. However, with the increase of temperature, the penetration depth gradually increases, reaching about 1.8 Å at 550 ℃. When the temperature reaches 550 ℃, the penetration depth jumps to a higher level compared to that of 500 ℃. Within the time scale (nanoscale) applicable to molecular dynamics, the number of O atoms going from the liquid LBE-O to the Fe substrate side is always about 1 as the temperature increases. At the initial stage of oxidation and dissolution of bcc Fe surfaces contacting with stagnant oxygen dissolved liquid lead-bismuth eutectic (LBE-O), the change in the number of O atoms going from the liquid LBE-O to the Fe substrate side is not so obvious in a short time as temperature increases, but the number of penetrating- atoms and the number of leaving- Fe atoms show a significant temperature effect when the temperature reaches 550 ℃. To better understand the interaction between dissolution

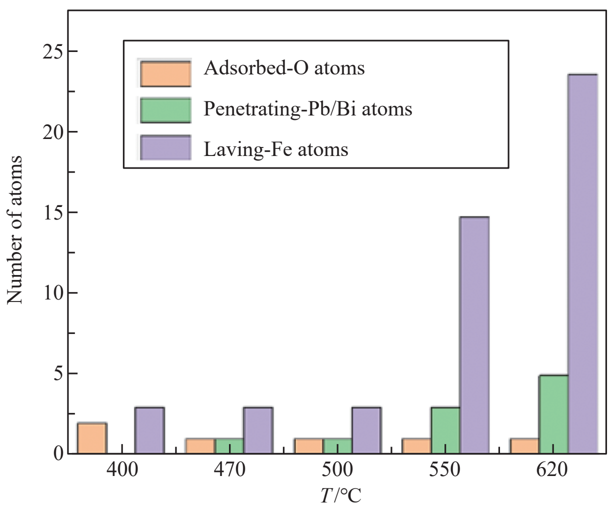

Fig. 1 (color online) Temperature dependent number of leaving-Fe atoms, penetrated- Pb/Bi atoms and adsorbed-O atoms

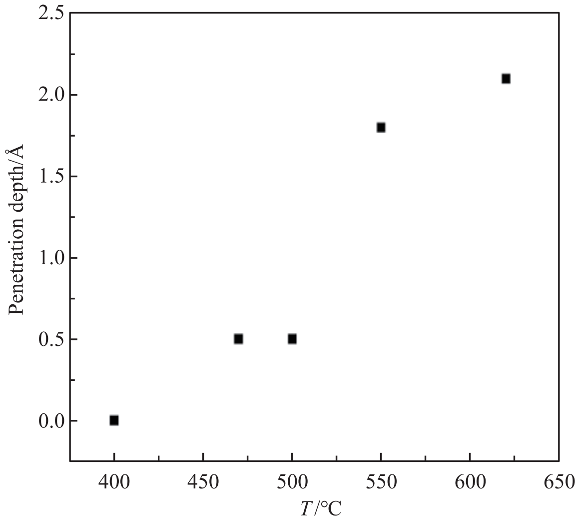

Fig. 2 Temperature dependent penetration depths of Pb/Bi atoms.

and oxidation, radial distribution functions (RDF) were used to characterize the structural evolution of the crystal surfaces during the oxidation. The results are shown in Fig. 3. With the increasing of temperature, the first peak intensity of Fe-O decreases gradually. The solubility of Fe atoms increases with the increasing temperature. It means that the Fe atoms are unstable even if they bond with O atoms when the temperature is high. Dispersion of the distance between Fe and O atoms makes it difficult for oxide to nucleate. The growth of oxides depends on the nucleation controlled by Fe-O bond and the continuous growth controlled by O atoms diffusion. Violent dissolution of Fe atoms makes it hard for oxide to nucleate when the temperature is 620 ℃.

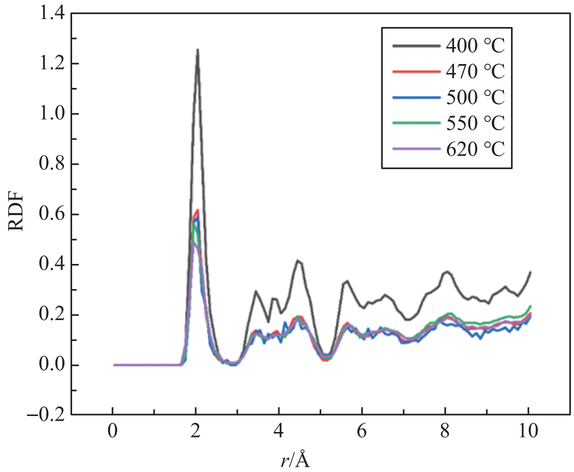

Fig. 3 (color online) Radial distribution functions for Fe–O pair obtained for Fe(100) surface at temperatures of 400, 470, 500, 550 and 620 ℃.

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