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Effect of Corrosive Liquid Lead Coolant on the Structural Stability of Iron Material

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Abstract. For the design of fast nuclear reactors, usually it uses the lead metal alloys for coolant materials. Researches about lead coolants, has been carried out experimentally. However, experimental studies in the nuclear material field, besides being expensive, usually also require high safety. In particular, research on the corrosive properties of liquid lead for structural materials requires serious treatment if carried out experimentally. In this case, the computational method is very helpful to overcome these obstacles. In our research we use the molecular dynamics simulation method to know the effect of temperatures and effect of liquid lead corrosion attack to iron material. We want to know that which one is most crucial that causing the damage of the materials: it is due to temperature or due to liquid lead attack. It has been observed from MSD curves of simulation results that the liquid lead can make iron material experiencing most damage if compared with temperature effect the interactions among atoms are described by the Lennard-Jonnes interaction potential. The simulations were run and supported using Moldy and Ovito software.

Keywords: Corrosion of molten lead, Fast nuclear reactor, Molecular dynamics simulation, Moldy, MSD, Ovito.

Introduction

The lead-cooled fast reactor is a nuclear reactor design that uses molten lead or lead-bismuth eutectic material as coolant. The most popular coolant as Lead-Bismuth Eutectic or LBE is a eutectic alloy of lead (44.5%) and bismuth (55.5%). In reactor physics and engineering, liquid metals are alloys with low melting points allowing for reactor coolant to be in liquid state in operating range of temperatures (above and not far from the room temperature) [1].

However, it is known that the liquid lead coolant is still a corrosive media, and without protection mechanism to the corrosion of steels from liquid lead attack then the application of nuclear coolant is not acceptable. Oxygen control technology has been developed to form protective oxide layers to increase the corrosion resistance of the steel exposed to liquid lead [2].

In addition to many studies related to corrosion prevention methods, there are also many studies to obtain superior corrosion-resistant new materials from molten lead [3]. It also has been found that the attack of molten lead on structural materials as a steel is qualifiedly related to the solubility of the solid in the lead [4].

Although a lot of research is experimental, computational research is often done to get details related to the microscopic state of the material. With computing things that are difficult to do

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experimentally are possible. In this case, molecular dynamics simulation methods and DFT (density functional theory) have received intense attention to be used in predicting the thermodynamic properties of nuclear materials such as liquid lead coolant [5-10]. Arkundato et al have used molecular dynamics methods to predict the thermodynamic physical properties of the corrosion phenomena of materials in molten lead metal [5-10]. Nuris (2019) also has studied the interaction of iron in liquid lead with variation of simulation geometry [11]. Imanullah et al have also worked on the molecular dynamics simulation to predict the temperature dependence of liquid lead density [12].

Although relatively many computational studies have been carried out, there are still many things that can be analyzed regarding the phenomenon of material corrosion to get a more comprehensive understanding of the symptoms of molten lead corrosion. In goal of the study is, we want to see how liquid lead actually affects materials, especially iron. Does iron work very fast when it interacts with molten lead? Is this damage purely due to temperature or is it due to interactions with the molten metal?

Theoretical Background

Classical molecular dynamics (MD) simulation is a computer simulation method for analyzing the physical movements of atoms and molecules based on the Newton equation of motion. The atoms and molecules are allowed to interact for a fixed period of time based on the certain interatomic potential, giving a view of the dynamic "evolution" of the system. In this research we used the Lennard-Jones potential to describe the interactions among atoms.

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \quad (1)$$

In this study we will see how strong the effect of molten lead on the breakdown of iron occurs. Simulation is done by placing iron in molten lead at a certain temperature and simulated by molecular dynamics method based on Lennard-Jones potential. The level of iron damage can be seen from the MSD (mean square displacement) curve of iron atoms dissolved in iron lead. The greater the MSD, the greater the damage to the material due to the high solubility of iron.

$$MSD \equiv \langle|x(t) - x_0|\rangle^2 = \frac{1}{N}\sum_{i=1}^{N}\left|x^i(t) - x^i(0)\right|^2 \quad (2)$$

In this study, we use the potential parameters to run the simulation those are $\varepsilon_{\text{Fe-Fe}}$ = 0.4007 (eV), $\sigma_{\text{Fe-Fe}}$ = 2.3193 Å, $\varepsilon_{\text{Pb-Pb}}$ = 0.1910 (eV), $\sigma_{\text{Pb-Pb}}$ = 3.1888 Å and $\varepsilon_{\text{Fe-Pb}}$ = 0.2766 (eV), $\sigma_{\text{Fe-Pb}}$ = 2.7541 Å [5].

Materials and Methods

In this study, we simulated the FePb interaction using the Moldy program developed by Keith Refson [13]. The temperature used for the simulations are in the range of 400-1100 K with a temperature increase of 200 K. We prepare the simulation for two goals:

1. Simulation of pure iron to know effect of temperatures to structure stability of iron
2. Simulation of iron in liquid lead to know effect of liquid lead to iron stability

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The stability of the iron will be seen from MSD curve [14]. The lower slope of MSD means the lower level of the iron damage.

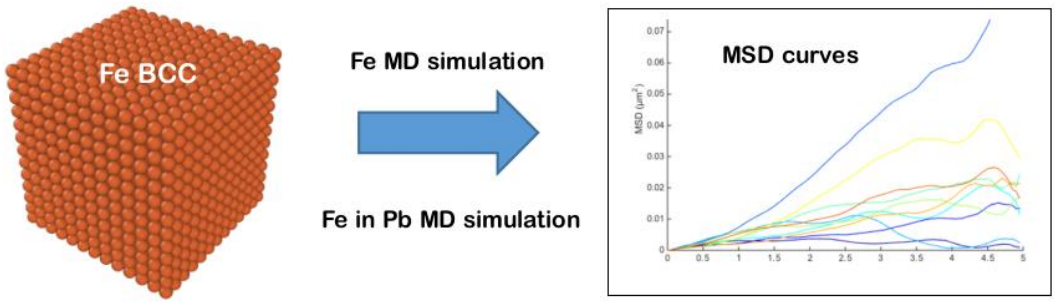

Figure 1. Scheme of MD Simulation of Iron

The number of atoms that simulated are iron 1729 (prepared in BCC crystal) and lead 5577 (prepared as liquid). The BCC iron was prepared by OVITO program [15].

Results and Discussion

The simulation results can be described in Figure 2 as below.

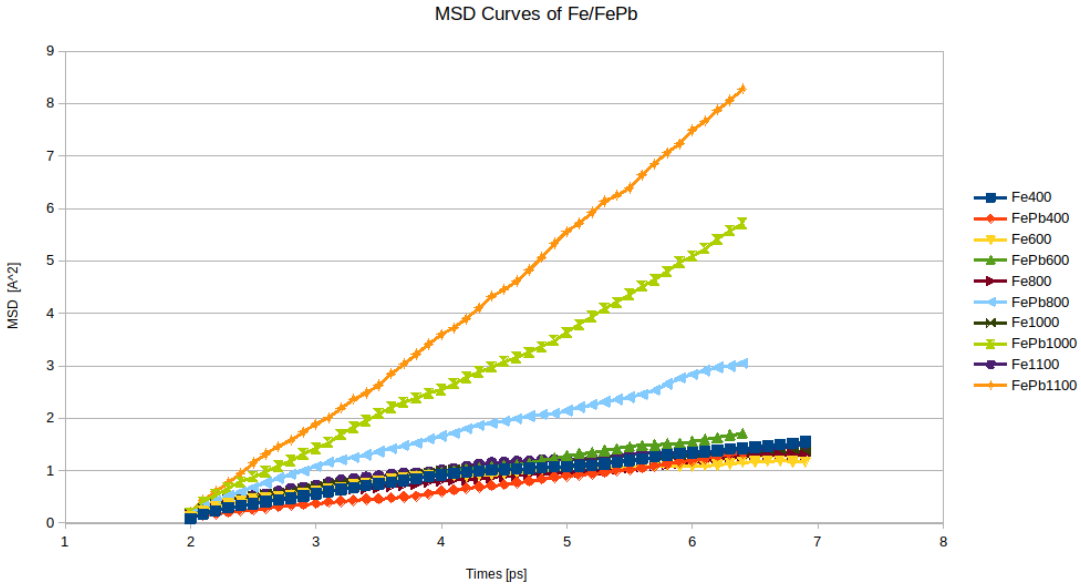

Figure 2. The MSD curves of Fe and Fe in Pb for several temperatures (400K, 600K, 800K, 1000K,1100K)

The MSD values were computed by previous above MSD formula. the top four MSD curves belong to the iron in the molten metal. Meanwhile, the bottom 4 curves that appear to clump

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together belong to iron without the influence of molten lead. We can see that temperature does affect the structure of the material. The higher the temperature, the faster the deterioration of the material.

However, from Figure 2 we can see that the molten lead metal effect greatly exacerbates the iron breakdown shown by the top four MSD curves. From Figure 2, we can see that the damage caused by temperature does not affect the structural damage of iron very quickly when compared to the damage caused by molten lead metal at various temperatures.

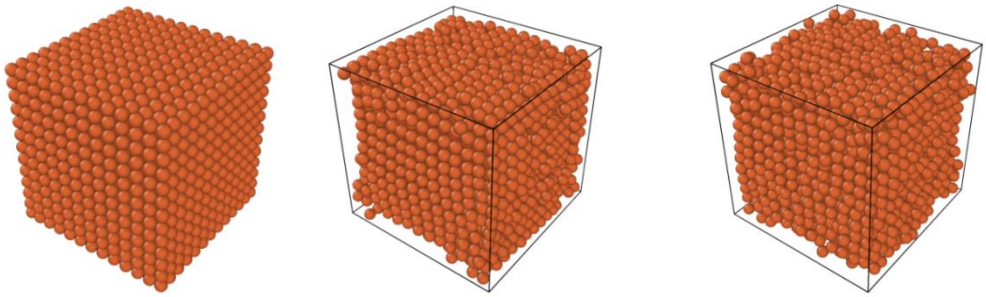

Figure 3. The structure of iron before and after molten lead metal attack: left (0K), middle (400K) and right (1000K)

Conclusions

From this study it can be concluded that the effect of temperature can cause material damage at high temperatures. But the effect of molten lead will cause far more damage than the effect of temperature. Therefore, if liquid lead is used as a coolant in nuclear reactor applications, it is necessary to look for superior materials that are resistant to damage either due to high temperatures or resistant to attack by liquid lead.

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