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Fe-Cr-Al-Ti STEEL FOR APPLICATIONS IN LEAD-COOLED FAST NUCLEAR-REACTOR DESIGN: A MOLECULAR DYNAMICS STUDY

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Abstract- Investigation of new potential materials for the development of the GEN IV "lead-cooled fast-nuclear-reactor design", has been carried out, computationally. One of the main problems of that design is the need to find materials that are heat resistant, corrosion-resistant from molten metal attack. This research is intended to find a proper composition of FeCrAlTi alloy steels that is resistant to high-temperature liquid lead corrosion. It is also, to inhibit this steel from high corrosion caused by liquid Pb, the oxygen with a very small concentration (0.199 wt.%) is also injected into the liquid lead. In this study we used computational molecular dynamics methods by applying strict procedures to find the exact composition and concentration of FeCrAlTi alloy steel. To research this steel, we looked for steel with the right composition and concentration based on the diffusion coefficient value and CNA (common neighbor analysis) value of the material. A large diffusion value indirectly indicates large corrosion/damage to steel in molten lead. Therefore, the material must display (look for) a diffusion coefficient that is as small as possible. It is known from the study, a promising candidate of corrosion-resistant steels in liquid lead is the steel with composition of Fe(77.45wt%) Cr(8.19wt%) Al(5.24wt%) Ti(9.12wt%). The same procedure can be applied to search for other new materials for other potential applications

Keywords: Liquid Metal, Steel Alloy, Molecular Dynamics, CNA, Corrosion Inhibition.

1. INTRODUCTION

The Gen-IV future reactor concept has been developed at the Generation IV International Forum to improve safety, sustainability, efficiency, and costs [1]. The Gen-IV reactor concept has 6 types of reactors, one of which is promising to be developed is a fast nuclear reactor cooled by liquid lead and/or lead-bismuth. However, it is known that besides having the very promising potential to be developed as a replacement for the previous type of traditional reactor (before Gen-IV), this liquid-lead cooled reactor design still contains many weaknesses that must be immediately overcome. The most challenging problem with the use of liquid lead is the presence of corrosion on the structural materials as cladding and the heat transfer pipe system in the reactor. Therefore, it is necessary to develop new or novel materials that are corrosion-resistant and also find an effective inhibition method of corrosion.

To inhibit corrosion, one method that is often applied is to introduce oxygen into this coolant with proper very small concentration [2]. There is a certain threshold concentration so that the oxygen supply can suppress the corrosion rate to the lowest limit, so that the reactor can be operated safely, efficiently, and economically [1]. All fast reactor designs operate at higher temperatures compared to older types, which frequently use water coolers. This operating temperature can even be more than 750 °C, so the cladding material or heat transfer pipe must be heat resistant as well as resistant to corrosion, caused by molten lead itself. Therefore, nowadays a lot of experimental and computational research has been carried out to find new, superior materials. Several new types of alloy steel have been developed such as 316LN austenitic stainless steel for reactor parts and pipe systems, 9Cr-1Mo steel for generator systems, and 9Cr-W-Ta RAFM steel also developed to obtain a better combination of strength and toughness [3].

Most recently, Peter, et al. have experimentally developed a FeCrAl alloy with the composition Fe-10Cr-4Al which was placed in a liquid lead medium at 750 °C. However, this material is said to still experience a certain amount of small oxidation [4]. Aluminum is also widely used as an alloy material for various technological applications where material characterization is very important [5].

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The development of new steel materials, the main alloy of 4 elements, is also being developed, such as FeAlCrTi steel. Capdevila, et al. have tested $Fe_2AlTi_{0.6}Cr_{0.4}$ steel at temperatures of 435 ℃ and 475 ℃, where Ti was added to obtain better mechanical properties [6]. Most material characterizations to see the potential of new steels for more promising applications, including the use of aluminum in steel alloys, often use tests on the mechanical properties of materials such as elastic modulus calculations [7]. At this point, it can be underlined that the development of new steels depends on many factors, for example: compositions of steel alloys, concentration of steel elements, temperatures, etc.

However, in this research we will not study the characteristics of materials based on measuring the mechanical properties of materials, but will look at the strength of materials against corrosion caused by liquid metal as a cooling medium in fast nuclear reactors. We want to find a new steel that is resistant to molten lead corrosion attack. There are several well-known agents that inhibit corrosion due to liquid lead, such as: oxygen, nitrogen, or others. Much experimental research has been carried out as described above, but with simulation methods research can provide initial prediction for discovery of new superior materials. A powerful simulation method that can be used is molecular dynamics (MD) [8-12]. Using this method, we observed the effectiveness of oxygen to suppress iron corrosion from molten lead attack.

One conclusion from the results of previous simulation work, there was a certain threshold concentration of oxygen that must be included in the lead (bismuth) coolant for minimum corrosion [9]. Then, we also studied the degradation of FeNiCr material [10]. We have also inspected the FeNiCrTi alloy steel using these molecular dynamics simulation method, and looked at its performance in molten lead based on existing compositions from other studies [11-12]. We carried out all these simulations using MOLDY software, which in our opinion has very good accuracy in calculating the diffusion coefficient [13].

In this current study, we still use the Lennard-Jones (LJ) potential to describe the interaction among atoms of materials. As an initial prediction, the use of the LJ potential makes the simulation work easier. We compute the diffusion coefficient of iron (in liquid lead coolant) to regard the corrosion phenomena. Furthermore, previously we also have developed a new formula for calculating the Lennard-Jones potential parameters for pairs of atoms of different elements to produce a more accurate diffusion coefficient of iron/metal in molten lead [13]. What is new in this study is that, with simulations we want to predict and determine what is the exact composition of each Fe, Cr, Al, Ti element in Fe-Cr-Al-Ti alloy steel that displays the best performance of corrosion-resistant steel in molten lead.

2. MOLECULAR DYNAMICS THEORY

Molecular dynamics technique is powerful for calculation of physical properties of material. Researchers have used this technique to predict the mechanical and structural of carbon nanotubes [14]. In our work, we used this technique to study the thermodynamic and structural properties of material. In molecular dynamics simulation, principally atoms that build up the materials will interact among them under certain potential energy $U(r)$ which is related to the force $F(r) = -dU(r)/dr$ in the conservative system. The dynamics of atoms is described by the Newton's second law of motion. We can use any types of potential energy function for specific purpose. We used the LJ potential for simplicity of calculation. The LJ potential is usually suitable for the liquid system, so it should be applicable also for the liquid lead [15]. The LJ (6-12) form can be stated as follows [16]:

$$U(r) = 4\varepsilon\left\{(\sigma/r)^{12} - (\sigma/r)^{6}\right\} \quad (1)$$

The parameter σ is in the length units, ε in the energy units. For a different type of elements A and B, especially for nonmetal, we can use the very popular Lorentz-Bertholet mixing formula for computing unsimilar pairs of atoms. For parameter σ We can use the rule proposed by Lorentz [17].

$$\sigma_{AB} = 0.5 \times \{\sigma_{AA} + \sigma_{BB}\} \quad (2)$$

while for the parameter ε we can use the rule proposed by Berthelot [18]

$$\varepsilon_{AB} = \sqrt{\{\varepsilon_{AA} \times \varepsilon_{BB}\}} \quad (3)$$

For metal systems, however we have developed the new mixing formula to compute σ and ε as in reference [11].

$$\sigma_{AB} = \left\{\sigma_{AA}^2 + \sigma_{BB}^2\right\}^{1/6} \quad (4)$$

$$\varepsilon_{AB} = \sqrt{\left\{\varepsilon_{AA}^2 + \varepsilon_{BB}^2\right\}} \quad (5)$$

Using both formulas all parameters of the LJ potential of FeCrAlTi in liquid Pb can be computed in Table 1.

Table 1. Parameter of LJ potential in our simulation [8-10, 21-23]

Pair of atoms	ε [eV]	σ [Å]	Annotation
Fe - Fe	0.5193	2.3193	as Ref. [8, 21]
Pb - Pb	0.2363	3.1888	as Ref. [8, 21]
Cr - Cr	0.6735	2.2813	as Ref. [10, 21]
Al - Al	0.0435	2.5735	as Ref. [22]
Ti - Ti	0.0330	2.6843	as Ref. [22]
O - O	0.0102	3.4280	as Ref. [8-9]
Fe - Pb	0.5705	1.5799	By Equations (4), (5)
Fe - Cr	0.8505	1.48175	By Equations (4), (5)
Fe - Al	0.5211	1.5131	By Equations (4), (5)
Fe - Ti	0.52035	1.52514	By Equations (4), (5)
Fe - O	0.07278	2.87365	By Equations (2), (3)
Pb - Cr	0.71376	1.5769	By Equations (4), (5)
Pb - Al	0.2403	1.6002	By Equations (4), (5)
Pb - Ti	0.23859	1.60936	By Equations (4), (5)
Pb - O	0.04909	3.3084	By Equations (2), (3)
Cr - Al	0.6749	1.5095	By Equations (4), (5)
Cr - Ti	0.67431	1.52159	By Equations (4), (5)
Cr - O	0.08288	2.85465	By Equations (2), (3)
Al - Ti	0.05460	1.54929	By Equations (4), (5)
Al - O	0.0211	3.001	By Equations (2), (3)
Ti - O	0.01835	3.0562	By Equations (2), (3)

2.1. Corrosion and Diffusion Coefficient

To see the effect of liquid lead on the damage to steel, we can look at the seepage of lead atoms into the steel, as was done by Alan, et al. [19]. However, not like Alan's research, we study corrosion as diffusion process. We want to watch Fe/Cr/Al atoms that dissolved into the liquid metal. We learn the corrosion/damage of the FeCrAlTi steel by monitoring the solubility of Fe/Cr/Al/Ti atoms into liquid lead. The quantity related to this solubility is the diffusion coefficient D [m^2/s]. Based on the Einstein relation, we can compute D as Equations (6), (7) [20]:

$$MSD = \left\langle \left| r(t) - r(0) \right|^2 \right\rangle = (1/N) \sum \left\{ \left| r^i(t) - r^i(0) \right|^2 \right\} \quad (6)$$

$$D = MSD / 6t \quad \text{(for 3D system)} \quad (7)$$

where, MSD is abbreviation of mean squared displacement. Following the above equation, the higher the diffusion coefficient D, the more corroded or damaged the steel material. Related to the FeCrAlTi material design we have to find the best composition of Fe-Cr-Al-Ti to provide the least corrosion or damage to the steel in a liquid lead environment.

3. METHOD

The procedure for obtaining steel alloy material FeCrAlTi with expected proper composition, namely Fe(a-wt%) Cr(b-wt%) Al(c-wt%) Ti(d-wt%) are as follows:

1. Prepare input of MD simulation: Fe in liquid Pb. The iron was prepared in a bcc crystal structure, composed of 10745 atoms Fe. The bcc Fe was placed in the center of liquid lead. Simulate the bcc-Fe crystal in liquid Pb with various oxygen content injected into liquid. Check and choose the most stable of iron crystal-structure, at a given oxygen content (x-wt%). This should be a proper oxygen concentration for minimum corrosion of FeCr steel and other.
2. Prepare input of MD simulation: FeCr steel material with a BCC (body-centered cubic) crystal structure in liquid lead material (with the addition of x-wt% oxygen that forms the Pb-O system). Prepare FeCr steel for various compositions of Fe and Cr to make alloys.
3. All MD simulations are carried out at temperature T = 750 °C with variations in the composition of Cr relative to the total mass of FeCr. From the simulation results (with x-wt% oxygen injected), we try to find out what concentration of Cr is capable of showing the most stable FeCr steel material (minimum corrosion) in liquid lead. At this stage, Fe(a1-wt%) Cr(b1-wt%) steel is obtained. The most stable FeCr steel for certain compositions in liquid lead if the diffusion coefficient of Cr is minimum.
4. MD simulation then is continued (at temperature T = 750 °C) with variations in composition by adding Al atoms to previous Fe(a1-wt%) Cr(b1-wt%) steel. From the simulation results, it will be obtained Fe(a2-wt%) Cr(b2-wt%) Al(c1-wt%) steel. The most stable FeCrAl steel for certain composition in liquid lead if the diffusion coefficient of Cr is minimum.
5. MD simulation then is continued (at temperature T = 750 °C) with variations in composition by adding Ti atoms to previous Fe(a2-wt%) Cr(b2-wt%) Al(c1-wt%) steel. From the simulation results, it is obtained at what concentration of Ti can show the most stable FeCrAlTi steel material (minimum or no corrosion). At this stage, the Fe(a3-wt%) Cr(b3-wt%) Al(c2-wt%) Ti(d1-wt%) steel is obtained, the expected FeCrAlTi that we are looking for. The results of this last simulation will show what steel alloys having good performance to resist liquid metal corrosion. This is the Fe(a3-wt%) Cr(b3-wt%) Al(c2-wt%) Ti(d1-wt%) steel. The most stable FeCrAlTi steel for certain compositions in liquid lead if the diffusion coefficient of Cr is minimum.

4. SIMULATION RESULTS

Now, we discuss about simulation results.

4.1. Determination of Oxygen Content in Liquid Lead

Simulation of Fe material in liquid Pb at temperature 750 °C with various number of oxygen atoms, was done to choose the best oxygen concentration for corrosion inhibition of iron. We can evaluate this in two ways: (1) by checking the most-stable structure of iron after simulation, and (2) by choosing the smallest diffusion coefficient of iron in liquid lead. In the first way, we compute the CNA (common neighbor analysis) of the iron material. We can do this by using OVITO code [23]. We check and choose the highest value of CNA of iron material. For the second way, we check and choose the smallest value of CNA of iron material. For the second way, we determine the lowest diffusion coefficient of iron in liquid lead. Figure 1 shows our simulation result, we can see that the injection of 1050 atoms (= 0.199wt%) of oxygen into 40685 Pb atoms (in liquid phase) shows, this is the best concentration of oxygen to stabilize the iron structure. This means the minimum corrosion of iron, that can maintain about 65.80% of iron still in the bcc structure.

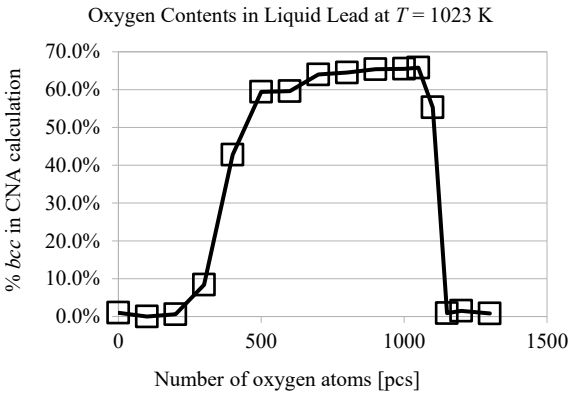

Figure 1. The relation between oxygen contents and CNA value

Example of the visualization of atoms of material before simulation, can be seen as in Figure 2. These two pictures we created by the Ovito program [23].

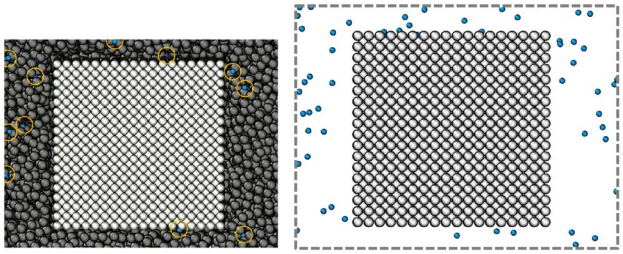

Figure 2. Slice of Fe-PbO system:
(left)-Fe in PbO system, (right)-Fe surrounded by oxygen
(Note: Fe = white grey, Pb = dark grey, O = cyan green color)

From simulations with various oxygen content, we can see and choose that, the injection of 0.199wt% oxygen into liquid lead will be able to maintain the iron stability (CNA = 65.8% of bcc structure). Figure 3 shows three images of the atoms of iron and one image of CNA calculation to know the structure type of material, using Ovito manipulation menu. All images were created using the Ovito program [23].

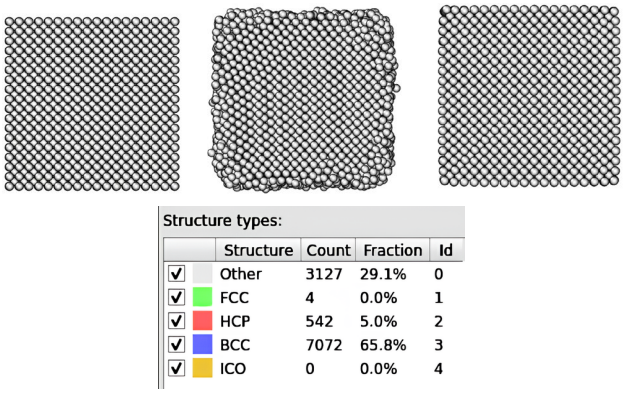

Figure 3. Iron structure: (top left)-before simulation, (top center)-after simulation without oxygen, (upper right)-after simulation with oxygen, (bottom middle)-CNA value

Empirical pictures how effective the oxygen for iron inhibition, can also be seen from solubility of iron. From the simulations, we can compute the diffusion coefficient for Fe in liquid Pb as in Figure 4.

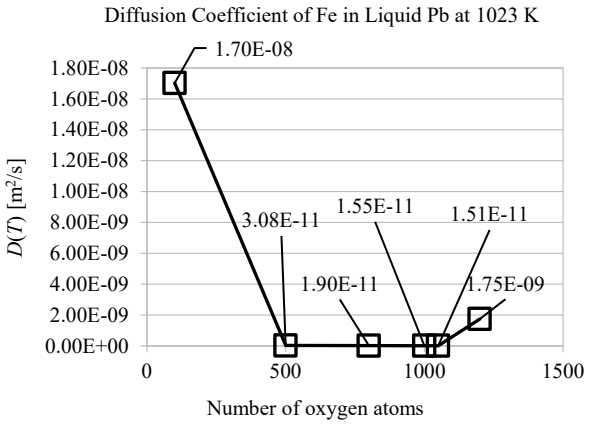

Figure 4. Diffusion coefficient of iron in liquid lead for different percentage of injected oxygen

From Figure 4, we can see that the lowest corrosion of iron to happen if the oxygen concentration is 0.199wt% (we use 40685 atoms of Pb (or (99.80wt%)) and 1050 atoms of Oxygen (or (0.199wt%)) to make Pb-O liquid system). Furthermore, injecting too little or too much oxygen will even cause more corrosion of the iron.

4.2. Finding a Proper Composition of FeCrAlTi

The new potential steels were researched by simulating various alloys with their own compositions. To inhibit corrosion, we also mix oxygen (0.199wt%) into molten lead. It should be emphasized here that the accuracy of the oxygen concentration is not the focus of the research, but the focus is how the composition and type of alloy determine the stability of the material in high-temperature molten lead, namely 750 °C. From the simulation, several important results can be seen as below.

4.2.1. Finding FeCr Steel

We started the work by preparing the FeCr steels with different compositions. To make FeCr steel with different compositions, we change some of Fe atoms (10745 initially) become Cr atoms for the certain number using the Atomsk code [24]. Figure 5 shows an example of Fe(9599) Cr(1145 = 10wt%) in lead liquid with oxygen (0.199wt%) for our input of simulation (images were created using the Ovito [23]).

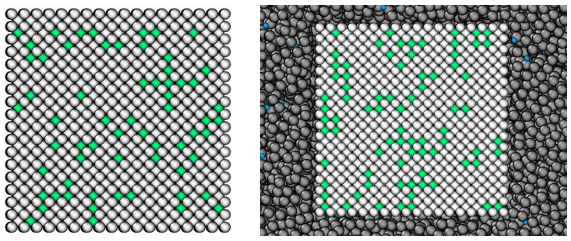

Figure 5. (left)-FeCr(10wt%), (right)-FeCr(10wt%) in PbO system
(Note: Fe = white grey, Cr = green, Pb = dark grey color)

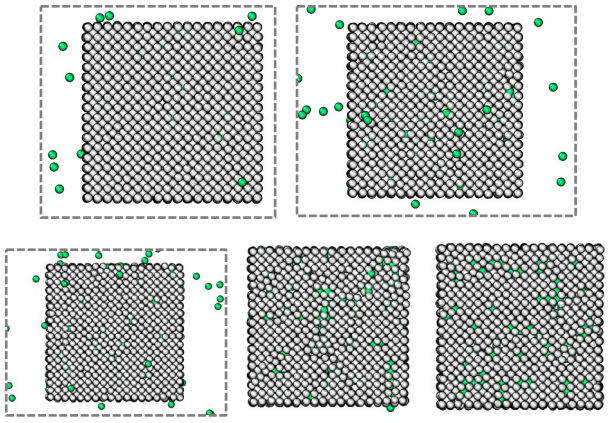

Figure 6. FeCr steel in liquid lead after simulation:
(top left)-Cr-3wt%, (top right)-Cr-6wt%, (bottom left)-Cr-8wt%, (bottom center)-Cr-9wt% and (bottom right)-Cr-9.56wt%
(Note: Fe = white grey color, Cr = green color)

MD simulation then was done for the 70,000-integration step using Beeman Algorithm in MOLDY code, at a temperature of 750 °C for several concentrations of Cr atoms. After simulation, we checked the structure of simulated FeCr using OVITO visualization code. The (small) concentrations of Cr atom in FeCr system were 3wt%, 6wt%, 8wt%, 9wt%, 9.56wt%. We found that the most stable FeCr structure in liquid Lead with oxygen if the steel composition was FeCr(9.56wt%). Figure 6 shows the visualization of FeCr with five compositions in liquid lead with oxygen (all images were drawn using the Ovito code [23]).

In Figure 6, the atoms of grey color are the Cr atoms. The Cr atoms that are outside of the brown area mean there is the degradation of steel, because there are atoms (Cr) detached from the surface of the metal. More Cr atoms move out, then more corrosion happens. We can see from Figure 6 that setting up the Cr concentration for only 3wt% shows the high dissolution of Cr atoms into the liquid lead. Setting up Cr for 6wt%, 8wt%, and 9wt% there is still dissolution of Cr atoms but it makes lower dissolution. Setting up Cr for 9.56wt% (Fe 9649, Cr 1096) seems stopping the dissolution of Cr atoms into the liquid lead. This investigation step concludes that the most stable structure for FeCr alloy steel in liquid lead is for composition of Fe(9649) Cr(1096) or exactly Fe(90.436wt%) Cr(9.564wt%). Clearly, the picture of effect of Cr concentration in FeCr steel can be seen from the diffusion coefficient calculation (Figure 7).

From Figure 7, we can see that the composition of Fe(9649) Cr(1096) or Fe(90.436wt%) Cr(9.564wt%) gives more structure stability of FeCr steel compared with other compositions.

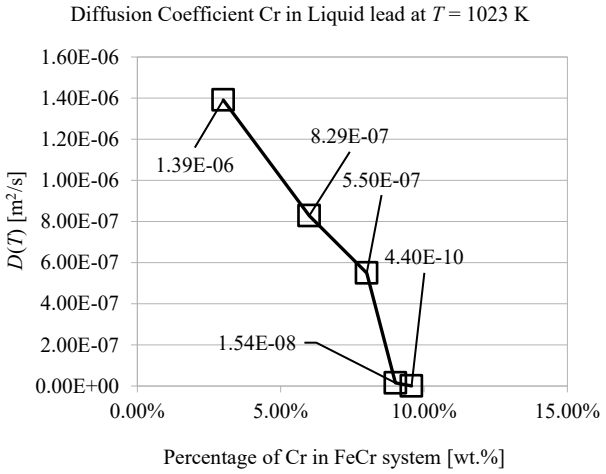

Figure 7. Effect of Cr concentrations to FeCr steel

4.2.2. Finding FeCrAl Steel

With a similar procedure to find Cr concentration in FeCr steel, now we add Al atoms to Fe(9649) Cr(1096) or Fe(90.436wt%) Cr(9.564wt%) steel. To do this we use the Atomsk code to make FeCrAl steel [25]. By various compositions of FeCrAl and simulating these steels in the liquid lead (PbO system) we had several important results. Figure 8 shows our simulation results for four different compositions of FeCrAl and its effects (All images were created using the Ovito code [23]).

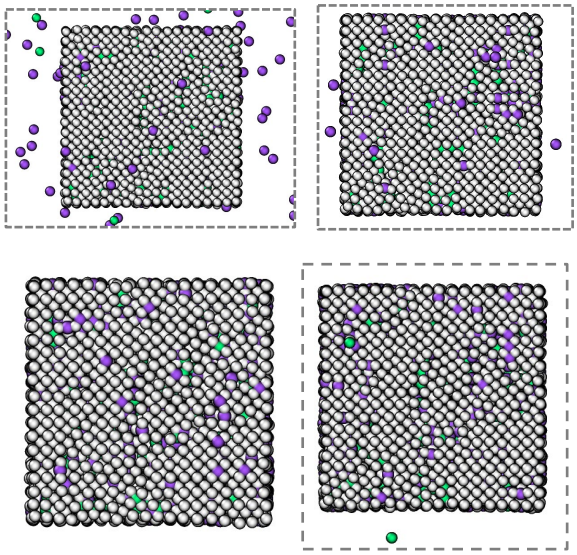

Figure 8. FeCrAl steel in the PbO system:
(top left) - Fe(86.411wt%) Cr(9.60wt%) Al(3.98wt%)
(top right) - Fe(85.96wt%) Cr(9.09wt%) Al(4.95wt%)
(bottom left) - Fe(85.22wt%) Cr(9.01wt%) Al(5.77wt%)
(bottom right) - Fe(83.24wt%) Cr(8.80wt%) Al(7.96wt%)
(Note: Fe = white grey, Cr = green, Al = purple color)

From Figure 8 (top left), adding atoms Al(3.98wt%) into Al(4.95wt%) to Fe(90.436wt%) Cr(9.564wt%) steel to make new steel it still shows high dissolution of Cr and Al atoms. Then in Figure 8(top right), adding Al(4.95wt%) to Fe(90.436wt%) Cr(9.564wt%) steel to make new Fe(85.96wt%) Cr(9.09wt%) Al(4.95wt%) steel, it still shows FeCrAl corrosion. From Figure 8(bottom left), we can also see that adding atoms Al(5.77wt%) to Fe(90.436wt%) Cr(9.564wt%) to make another new Fe(85.22wt%) Cr(9.01wt%) Al(5.77wt%) steel, it shows no high dissolution of Fe/Cr/Al atoms (corrosion) into lead liquid.

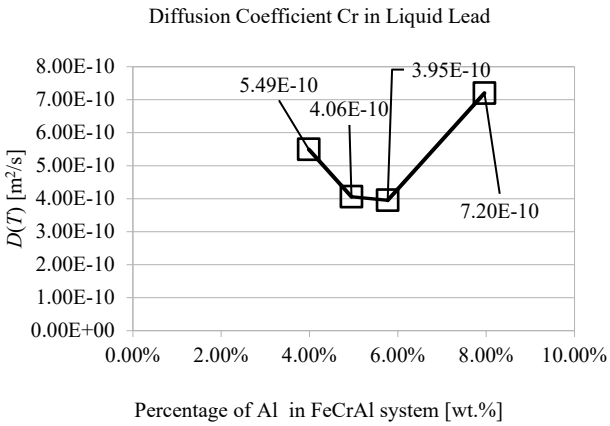

Figure 9. Effect of Al concentration to FeCrAl steel

However, adding more Al atoms is about 7.96wt% to build Fe(83.24wt%) Cr(8.80wt%) Al(7.96wt%) steel, it will appear again the dissolution of Al atoms (Figure 8 (bottom right)).

So, proper composition of FeCrAl steel for usage in molten lead environment, it should be Fe(85.22wt%) Cr(9.01wt%) Al(5.77wt%) steel. Clearly, picture of the effect of Al concentration in FeCr steel can be seen from the diffusion coefficient calculation, Figure 9. From Figure 8, we see that the Cr atoms more easily dissolved compared to other atoms Fe and Al into liquid lead. Figure 9 shows the diffusion coefficient of Cr in liquid lead for every percentage of Al atoms in the FeCrAl steel system. We can see that, the most stable of the FeCrAl steel in liquid lead if the composition of the steel is about Fe(9649) Cr(1096) Al(1352) or Fe(85.22wt%) Cr(9.01wt%) Al(5.77wt%), where this presents the smallest Cr diffusion coefficient.

4.2.3. Finding FeCrAlTi Steel

Now, we add Ti atoms to build FeCrAlTi steel from Fe(85.22wt%) Cr(9.01wt%) Al(5.77wt%) steel to build a new steel. With a similar procedure we create several FeCrAlTi with different compositions and do corrosion simulation in a liquid lead system. Figure 10 shows the pictures of the simulation results (All images were visualized using the Ovito code [23]).

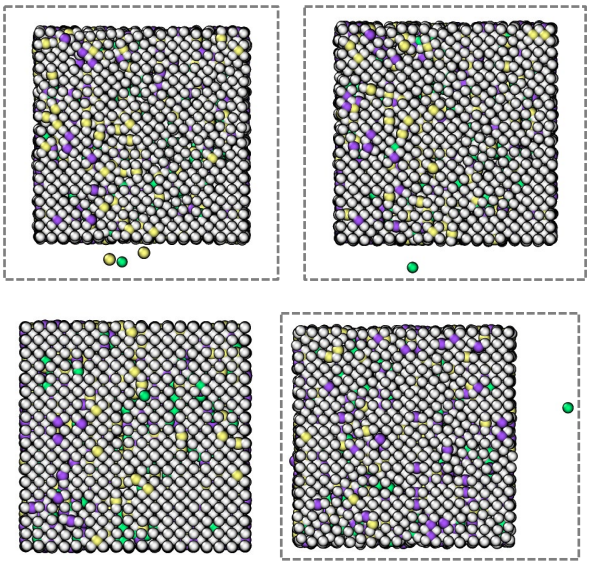

Figure 10. FeCrAlTi (Fe-brown, Cr-blue, Al-dark grey):
(top left) - Fe(77.97wt%) Cr(8.27wt%) Al(5.28wt%) Ti(8.50wt%)
(top right) - Fe(77.50wt%) Cr(8.20wt%) Al(5.25wt%) Ti(9.05wt%)
(bottom left) - Fe(77.45wt%) Cr(8.19wt%) Al(5.24wt%) Ti(9.12wt%)
(bottom right) - e(76.68wt%) Cr(8.11wt%) Al(5.19wt%) Ti(10.01wt9%)
(Note: Fe = white grey, Cr = green, Al = purple, Ti = yellow color)

From Figure 10 (top left), the addition of 1227(=8.50wt%) Ti atoms to the previous steel Fe(85.22%) Cr(9.01%) Al(5.77%) to make a new steel Fe(77.97wt%) Cr(8.27wt%) Al(5.28wt%) Ti(8.50wt%), this actually shows high dissolution of Cr(green) and Ti(yellow) atom into liquid lead. Then Figure 10 (top right), the addition of 1315(=9.05wt%) Ti atoms to the previous steel Fe(85.22%) Cr(9.01%) Al(5.77%) to make new steel, Fe(77.50wt%) Cr(8.20wt%) Al(5.25wt%) Ti(9.05wt%), this still shows dissolution of Cr/Al into the molten lead (the atoms outside of white grey area is Cr and Al). Then from Figure 10 (bottom left), the addition of Ti atoms 1326(=9.12wt%) to make a new steel Fe(77.45wt%) Cr(8.19wt%) Al(5.24wt%) Ti(9.12wt%), it shows that there is no high dissolution of Fe/Cr/Al/Ti atoms into the molten lead. The steel composition of the Fe(77.45wt%) Cr(8.19wt%) Al(5.24wt%) Ti(9.12wt%) shows more stability in the PbO liquid system. From Figure 10 (bottom right), adding more Ti atoms, 1470(=10.01wt%) to make or build a new steel Fe(76.68wt%) Cr(8.11wt%) Al(5.19wt%) Ti(10.01wt9%) shows the presence of dissolved Cr into the molten lead again. So, this steel structure is less stable.

Clearly, physical picture of the effect of Ti to FeCrAl steel, it can be seen from the diffusion coefficient profile, as in Figure 11.

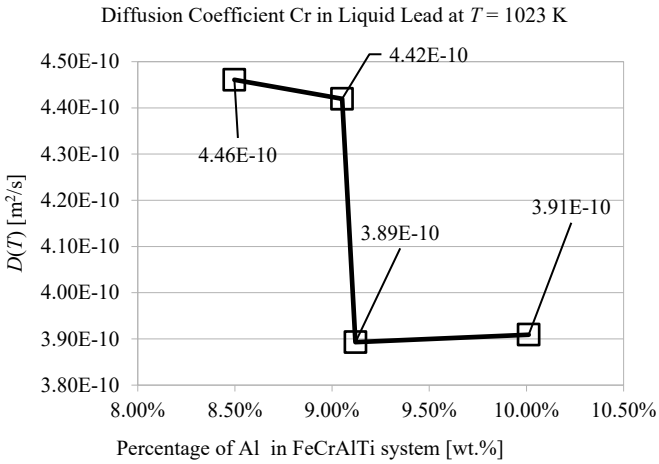

Figure 11. Effect of Ti concentration on FeCrAl steel

From Figure 11, we can note that the lowest diffusion coefficient of Cr is D_{Cr} = 3.89E-10 m^2/s, belongs to Fe(77.45wt%) Cr(8.19wt%) Al(5.24wt%) Ti(9.12wt%). The diffusion coefficient was computed using Equation (7). So, the potential of FeCrAlTi steel for the use in lead-cooled fast nuclear reactor design is for temperature of 750 °C is Fe(77.45wt%) Cr(8.19wt%) Al(5.24wt%) Ti(9.12wt%). For other temperatures, maybe this composition is still relevant although continued research must be done.

4.2.4. General Discussion

It is known that a ferritic SS (>12%Cr) steel is not currently used as structural materials for commercial reactors [25]. Our simulation work has shown that the composition of FeCr steel for the use in molten lead is Fe(90.436wt%) Cr(9.564wt%). So, the computational result is in accordance with that existing experimental data. Researcher also studied experimentally, the steel FeCrAl for accident tolerant fuel cladding materials with Al contents of 5.26wt% [26]. Our simulation shows the steel is Fe(85.22wt%) Cr(9.01wt%) Al(5.77wt%). The research has also investigated the Fe–13Cr-5Al-0.3Ti alloy in air, but not in molten lead [27]. Our simulation has shown that the steel for use in molten lead is Fe(77.45wt%) Cr(8.19wt%) Al(5.24wt%) Ti(9.12wt%). We need more titanium for safety use in fast nuclear reactor application.

5. CONCLUSIONS

From the results of molecular dynamics simulations, we can see that, by carrying out the procedure of adding each metal element one by one at different concentrations, starting from adding Cr atoms to Fe to get FeCr steel, adding Al atoms to FeCr to get FeCrAl material, then Ti atoms to FeCrAl to get FeCrAlTi steel, we can look for steel with the most appropriate composition which produces FeCrAlTi steel which is corrosion resistant in liquid lead at a certain temperature. It can be concluded from current simulation work that, the promising FeCrAlTi steel used in molten lead environments such as in the case of molten lead-cooled fast nuclear reactors is Fe(77.45wt%) Cr(8.19wt%) Al(5.24wt%) Ti(9.12wt%) steel. In this study, the steel is predicted to be operated at temperature 750 °C. We analyze the performance of FeCrAlTi based on the diffusion coefficient of atoms Cr chromium dissolved into molten liquid lead, applying corrosion inhibition by injecting oxygen with a concentration of 0.199wt% into liquid lead. This strict procedure makes it possible to find other alloy steels in various types of reactor cooling media or for other technological applications.

NOMENCLATURES

1. Acronyms

CAN	Common Neighbor Analysis
MOLDY	Name of molecular dynamics program
MSD	Mean Square Displacement
OVITO	Name of visualization program
PbO	Liquid lead with oxygen injection

2. Symbols / Parameters

T: Temperature
t: Time
D: Diffusion Coefficient
r: Position or distance
F: Force
U: Potential Energy
ε : Depth of LJ Potential
σ : Repulsion Distance
m: Mass of Atom

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