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# MOLECULAR DYNAMICS SIMULATION OF CORROSION AND ITS INHIBITION: COMPARISON OF STRUCTURAL STABILITY OF Fe/FeNi/FeNiCr/FeNiCrTi STEELS UNDER HIGH-TEMPERATURE LIQUID LEAD

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**Abstract**

The liquid lead used in fast nuclear reactor has been known to be able to cause a significant damage to the steels. Therefore, finding new materials with high corrosion resistance is the goal of much research current days. Likewise, developing a way to prevent corrosion is also the goal of designers of nuclear reactors. In the present study, we studied materials: Fe, FeNi, FeNiCr, and FeNiCrTi (a type of SS 316L austenite steel), comparing their structural stability when interacted with molten liquid lead at 750 °C. The performance of each steel is compared under high-temperature molten lead coolant, checking the structure's stability to see the material resistance to corrosion attack of liquid lead. The corrosion can also be seen from the data of iron diffusion coefficient. The larger of the iron diffusion coefficient can be associated with larger corrosion because there is a high solubility of iron atoms from the steel surface to the molten lead. The popular way to prevent more corrosion is by injecting oxygen into the lead coolant. This current work uses the molecular dynamics method to simulate the corrosion and inhibition phenomena. The research aims to compare the performance of Fe, FeNi, FeNiCr, and FeNiCrTi under liquid lead at a temperature of 750 °C. The diffusion coefficient of iron of material will be calculated to describe quantitatively the corrosion level of those structural materials and the corrosion inhibition by oxygen injection. The study has produced important results that adding Ni, Cr, Ti into a pure iron crystal to build alloy steel will make the material stronger, structurally compact, and more resistant to corrosion. For specific composition of steels, from weaker to stronger that resist from corrosion attack, it is possible to make ordering: Fe ≪ FeNi < FeNiCr < FeNiCrTi. The composition of FeNiCrTi steel in this work is Fe(75)Ni(10.57)Cr(14.05)Ti(0.40). The high corrosion of FeNiCrTi in the liquid lead is effectively reduced by injecting 0.0112 wt % oxygen into lead coolant as a limit value for maximum corrosion inhibition.

**Keywords:** Steels, liquid metal corrosion, diffusion, inhibition, molecular dynamics, oxygen injection.

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## 1. Introduction

Nuclear material research for reactor designs has obtained much attention in current days. Primarily for fast nuclear reactor design where the coolant material is liquid metals. The liquid metal-cooled fast reactors (LMCFR) have many benefits as a generation-IV nuclear reactor for the future. However, it still has a major problem for application, i.e., the structural material that is used in the reactor seems to experience high corrosion by interaction with liquid metals coolant as a lead liquid. To solve this problem, at least there are two crucial issues: (1) finding new novel materials and (2) looking for a way to inhibit corrosion. Many researchers have tried to find new, better steel alloys and investigate available or new materials with a ceramic structure. They try to find new corrosion-resistant material, resistant from high corrosion attack of liquid metal. They looked for new ceramics for high-temperature applications.

Research on nuclear materials and corrosion has been carried out based on the above issues. It has been reported the experimental corrosion of Liquid lead on the structural steels for their application in fast nuclear reactors design or accelerator-driven transmutation systems. It was needed to know how to mitigate the corrosion of the structural materials. One approach for the anti-corrosion is to use the traditional oxygen injection to maintain a protective oxide film on the surfaces of the structural materials by carefully controlling the oxygen concentration in the lead at a sufficient level. The solubility of steel components such as iron, chromium, and nickel in the liquid lead also plays an important role in the corrosion processes. The experimental result shows that the solubility of Ni in the liquid lead is much higher than that of Fe and Cr. The different solubility of the materials leads to selective dissolution and intergranular corrosion, which may eventually cause structural materials' failure [1].

It is also investigated the performance of Fe-10Cr-4Al alloys exposed to liquid lead at 750 °C for up to 1970 h to look for a better material for LMCFR application. The experimental alloys were based on the 10 wt % Cr and 4 wt % Al composition [2].

It is also reported the experimental results about the microstructure of an alumina-forming austenitic stainless steel with a composition design of Fe-18Ni-16Cr-4Al-2Mo-0.4Nb (in wt/ %) in the static liquid lead, with the different oxygen content of injection to prevent corrosion at 700 °C [3].

The other experimental study was about the 10Kh15N9S3B1 (EP-302) austenitic steel with fcc structure for the elements of the main equipment, which operated in contact with lead coolant to a maximum temperature 550 °C [4].

Several steels, for example, T91 and EP-823, were also studied by exposing them to either static or flowing liquid lead-bismuth eutectic under various exposure conditions about 500 °C to 550 °C. The T91 steel has a composition of Cr 8.99 wt % and Ni 0.11 wt %, and EP-823 steel has a composition of Cr 11.70 wt % and Ni 0.66 wt % [5].

A new promising material candidates for LMCFR was also studied in the year 2021. The adjustment of the Cr content in the FeCrAl alloy is one of the effective ways to obtain an enhanced performance for the FeCrAl alloy. They reported that compared with Al content, Cr content has less effect on Fe-xCr-6Al oxidation resistance [6]. At this stage, it is undeniable that until now, even research on new materials for fast nuclear reactor design and applications is still a very interesting research topic. Latest, in the year 2022 have been reported the investigation of T91 type of steels to be used in the liquid lead [7].

The last report about the experimental result of liquid metal corrosion was the behavior of refractory metals in the liquid lead at 1000 °C for 1000 h. In this study the corrosion behavior of some refractory metals (Nb, Nb521, and Mo-0.5La) was investigated in the static lead at 1000 °C for 1000 h [8].

An important point underlined from the above experimental studies is that the research of new materials that are corrosion resistant to molten lead is still a very interesting subject today. Even the alloy steel materials studied are still alloy steels of Fe, Ni, Cr, and Al components.

Nowadays, simulation researches have become a trend to complement experimental research. With simulation, many important conclusions can be predicted which is experimentally difficult. For example, is an effort to find a way of corrosion inhibition by using a popular technique of oxygen gas injection into the liquid metal with proper concentration. Experimentally, it is certainly not

easy to find out what is the right oxygen concentration for maximum inhibition of corrosion of steel or structural materials in molten lead metal, especially at very high temperatures above 750 °C. Using computational methods, especially the molecular dynamics (MD) simulation method then using correct inputs of simulation, many physical properties that describe physical phenomena such as corrosion can be predicted with accuracy that can be improved. Then, related to the materials to be used in liquid metals, it can be searched what's new material that having high performance resistant to molten metal corrosion.

The simulation research of FeNiCr steel cladding has been studied simulated at a medium temperature of 300−500 °C, not immersed in a liquid lead coolant but for a supercritical water-cooled reactor (SCWR) [9]. Also, as in our previous work, the molecular dynamics simulation method was used to research the liquid metal corrosion phenomena [10−12]. This simulation method is very powerful in predicting thermodynamics and mechanical properties of materials, for example, the diffusion coefficients. This coefficient can describe the material's resistance from corrosion attacks of liquid metal. As iron is a major component of steel, that molecular dynamics simulation can calculate how high the iron atoms will dissolve into liquid metal due to corrosion. With the molecular dynamics method, it is possible to design new materials with a new composition of different elements (alloys) that resist high liquid metal corrosion. The molecular dynamics method can predict the proper oxygen concentration for the best corrosion inhibition.

In our previous work, the performance of FeNiCr steel in the liquid lead by MD method was also investigated [13]. The corrosion of FeNiCr steel was examined by measuring the diffusion coefficient of iron inside the molten lead metal. In this study, we tried introducing oxygen into the liquid lead at a certain concentration. The oxygen concentration that inhibiting iron corrosion in FeNiCr materials can be simulated. The most minimum FeNiCr corrosion can be seen from the least diffusion coefficient of iron. Next, cast irons can be alloyed with strong carbide-forming elements such as Ti, V, Nb, and Mo to increase resistance [14].

Our current research is simulation work, where it is possible to study several steel alloys for application in a liquid lead environment. Let's compare the performance of Fe, FeNi, and FeNiCr materials and add Ti elements to see the performance of FeNiCrTi alloy steels when interacting with molten lead metals. Our objective of current research is to see the material's performance from the corrosion attack of molten lead metal and its inhibition. Let's measure the diffusion coefficient of iron in every steel alloy (Fe/FeNi/FeNiCr/FeNiCrTi) before and after being given an oxygen inhibitor into a liquid lead coolant. In the study, it is possible to see the effect of oxygen injection on corrosion inhibition and also see whether the addition of elements of Ni, Cr, and Ti elements had an impact on the stability of the material structure. Let's simulate the corrosion phenomena at a high-temperature condition, 750 °C.

## 2. Materials and Methods

### 2. 1. Materials

In molecular dynamics simulation, material atoms interact with a specific potential energy. By using the relation, $F = -\nabla U(r)$ for the conservative system, all atoms will follow Newton's law of motion $F = dp/dt$. Depending on the materials under consideration, the specific potential energy is usually used to describe the interaction among atoms, for example, the Lennard-Jones, Morse, EAM potential, etc. Depending on the research goal, the specific potential is used to describe the phenomena accurately. For our corrosion study of the metal system (FeNiCrTi-PbO), for easy calculation, let's use the Lennard-Jones (LJ 12-6), which is the very popular one that is also used by other researchers [15]. This LJ potential may not be so accurate for the metal system. But for simple calculation, getting qualitative research results may be very useful and important. In addition, our corrosion system is a mixture of solid (Fe-Ni/Cr/Ti) and liquid (Pb), and also gas (Oxygen); using the Lennard-Jones potential for investigating the corrosion phenomena may be quite reasonable.

Our current work will perform molecular dynamics simulation using the Moldy program/code [16]. This code is old software created in the year 2000, but according to researchers, it is still relevant to be used for doing research. This code is very accurate for calculating the pro-

perties and may use the Beeman algorithm for numerical integration. The Lennard-Jones potential (with parameters σ and ε) used in this study using the data for the metal system that have been tabled [17]. The LJ (12-6) can be written as follows:

$$U(r)=4\varepsilon[(\sigma/r)^{12}-(\sigma/r)^{6}], \quad (1)$$

where σ is in unit Å, and ε is in unit eV. This type of potential function was also used by some researchers to simulate the traveling distance of Pb atoms into FeNiCr material [18]. However, they didn't calculate the diffusion coefficient of the material where the diffusion process occurs.

**2. 2. Methods**

All simulations for corrosion investigation will be done under the Moldy molecular dynamics program [16]. The corrosion will be investigated by seeing the diffusion coefficient of iron, i.e., the major steel component, in the liquid lead. The bigger the diffusion coefficient of the Fe atom, the heavier the corrosion occurs. In this study, we are looking for a new material with the lowest diffusion coefficient of iron when steel material is immersed in the liquid lead at a high temperature of about 750 °C or 1023 K. Let's compare the diffusion coefficient of Fe of four materials: pure iron (Fe), FeNi, FeNiCr, and FeNiCrTi. It is possible to observe how resistant the material is under high-temperature liquid lead, which is indicated by the small value of the iron diffusion coefficient of every steel when inside the molten lead. The procedure to compute the coefficient diffusion can be seen as in **Fig. 1**.

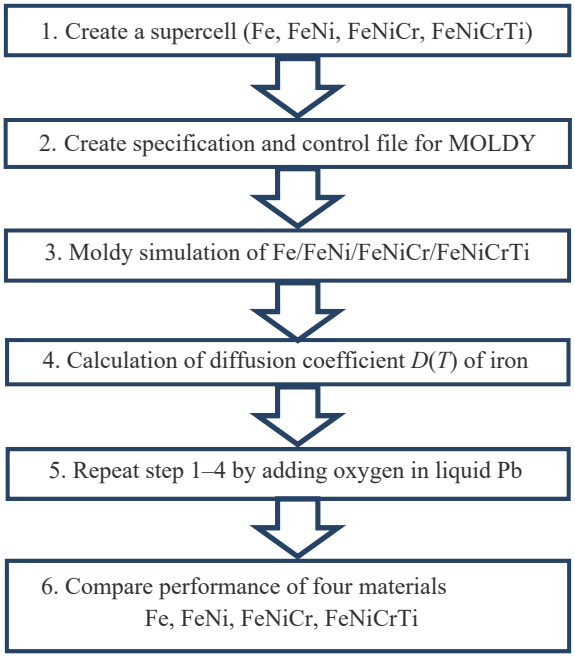



**Fig. 1.** Procedure of corrosion and inhibition simulation

In this procedure, simulation with oxygen will be done with different concentrations. This work is to study the effect of oxygen injection on corrosion inhibition. It is possible to look for the best concentration of oxygen that should be injected into the liquid lead to inhibit the steel corrosion maximally.

**2. 2. 1. Building supercell: steel materials and corrosion system**

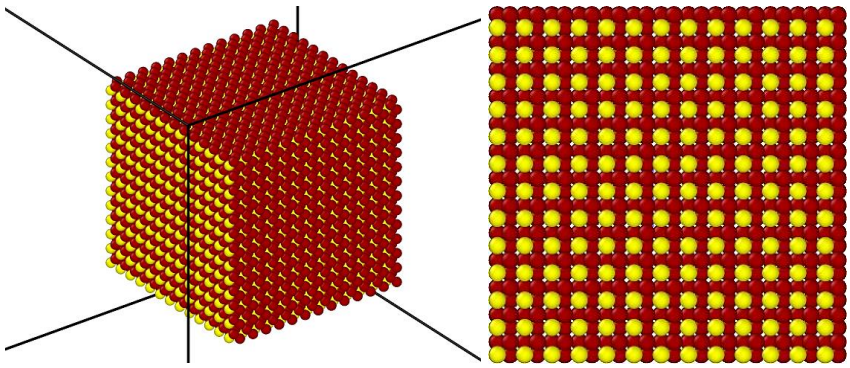
The simulation of Austenite SS316 steel starts with building a FeNiCr material system. Let's start with choosing the unit crystal of FeNi. The unit crystal of FeNi material is as following the *xyz* input file [19]:

```
#FeNi.init
4
5  #FeNi --- structure FCC a = 3.49869656 Å
Ni 0 0 0
Fe 1.74934828 1.74934828 0
Fe 1.74934828 0 1.74934828
Fe 0 1.74934828 1.74934828
```

To make the supercell of the feNi system, let's duplicate this unit crystal for the 13×13×13 dimension by using the «ATOMSK code» command line [20]:

```
$atomsk FeNi.init --duplicate 13 13 13 FeNi_13x13x13.xyz.
```

This input will make the supercell of the FeNi material system with 8788 atoms. The crystal structure of FeNi_13x13x13 with dimension 46.742 Å is described in **Fig. 2.** Then, let's observe the performance of this FeNi_13x13x13 material under the influence of liquid lead metal by MD simulation. Put the FeNi_13x13x13 in the center of 123×124×125 $Å^3$ of liquid Pb. The separation distance between Fe/Ni and Pb equals 2.7541 Å (similar to the $\sigma_{Fe\text{-}Pb}$ parameter of Lennard-Jones potential). The FeNi_13x13x13 in liquid Pb structure was set up using the Ovito modification utilities [21].



*a* *b*

**Fig. 2.** The FCC FeNi: *a* – 3D view; *b* – 2D view (brown = iron; yellow = nickel)

The simulation procedure of this material corrosion system (as **Fig. 1**) is implemented in the below-detailed steps:

1. Make the liquid lead system (by Moldy simulation) of temperature 750 °C with the dimension of about 123×124×125 $Å^3$. The temperature of 750 °C or 1023K is the temperature where let's observe the corrosion. Then there is the Pb_123x124x125.xyz file.

2. Open the file Pb_123x124x125.xyz by using Ovito code, use the modification utility and select the particles manually by logical command: 37.2815 < Position.X&&Position.X < 89.5312&&37.2815 < Position.Y&&Position.Y < 89.5312&&37.2815 < Position.Z&&Position.Z < 89.5312 (then delete the selected particles). This file will make an empty space in the center of Pb_123x124x125.xyz. Give the name of this new Pb_123x124x125.xyz as Pb_hole.xyz.

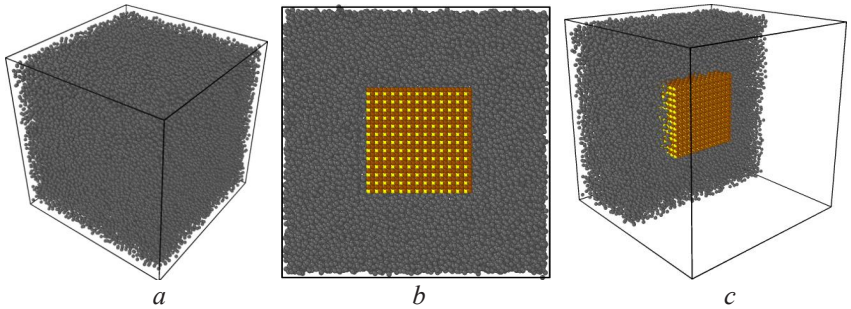
3. Combine the FeNi_13x13x13.xyz file and Pb_hole.xyz file by using Ovito modification or manually. It means we combine the coordinates of atoms of these files into one file material system. Then there is a picture of FeNiPb, as shown in **Fig. 3** below.

4. Simulate this FeNi in Pb liquid system using Moldy program following the specification file with an appropriate format as below:

```
#FeNiPb.in
iron 6591
1 0 0 0 55.847 0 Fe
```

```
lead 45134
2 0 0 0 207.19 0 Pb
nickel 2197
3 0 0 0 58.6913 0 Ni
end
lennard-jones
1 1 0.4007 2.3193 #Fe Fe # Following reference [17]
2 2 0.1910 3.1888 #Pb Pb
3 3 0.3729 2.2808 #Ni Ni
1 2 0.2766 2.7541 #Fe Pb #Computed by Lorentz-Bertholet formula [15]
1 3 0.3865 2.3001 #Fe Ni
2 3 0.2668 2.7348 #Pb Ni
end
123 124 125 90 90 90 1 1 1
lead 0 0.363301 0.740768
.....
lead 0.001937 0.653934 0.95968
.....
nickel 0.69128 0.685708 0.68022
.....
iron 0.691283 0.699815 0.694217
end
```

As mentioned above, specification data of material and the potential parameters of different elements were computed by using the Lorentz-Bertholet mixing formula [15].



*a* *b* *c*

**Fig. 3.** The FeNiPb system: *a* − outside view; *b* − front view of slice; *c* − side view of slice (gray = lead; brown = iron; yellow = nickel)

Then, all simulations of the corrosion and inhibition investigation will be done by controlling the Moldy simulation as the control file below.

```
const-temp=1            # Nose_Hoover Thermostat
temperature=1023        # Kelvin
const-pressure=4        # Andersen constant pressure
nsteps=50000            # integration step
step=0.0001             # timestep
end
```

In the meantime, it is also necessary to compare the FeNiPb system with FePb system. It is necessary to observe whether our FeNi system is more stable than the Fe system when it is immersed in the liquid lead. For the FePb system, let's change all Ni atoms to Fe atoms. To create a FeNiCr material system, it is possible to manipulate the previous FeNi structure. The FeNiCr material system for corrosion simulation can be described in **Table 1** below.

**Table 1**
Composition of FeNiCr steel

| Element | # atoms | mass/atom | total masses | wt s% in FeNiCr |
|---|---|---|---|---|
| Fe | 6591 | 55.847 | 368087.577 | 75.40 |
| Ni | 879 | 58.6934 | 51591.4986 | 10.57 |
| Cr | 1318 | 51.9961 | 68530.8598 | 14.04 |

The input (specification) file of Moldy simulation the is like:

```
#system FeNiCr.in
iron 6591
1 0 0 0 55.847 0 Fe
lead 45006
2 0 0 0 207.19 0 Pb
nickel 879
3 0 0 0 58.6913 0 Ni
#oxy 40
#4 0 0 0 15.999 0 O
chrom 1318
5 0 0 0 51.9961 0 Cr
end
lennard-jones
1 1 0.4007      2.3193      #Fe Fe [17]
2 2 0.1910      3.1888      #Pb Pb
3 3 0.37289     2.28080     #Ni Ni
#4 4 0.01020    3.42800     # O O
5 5 0.41295     2.33570     #Cr Cr
1 2 0.2766      2.7541      #Fe Pb #Computed by Lorentz-Bertholet rules [15]
1 3 0.3865      2.3001      #Fe Ni
#1 4 0.06393    2.87365     #Fe O
1 5 0.40678     2.32750     #Fe Cr
2 3 0.2668      2.7348      #Pb Ni
#2 4 0.04413    3.3084      # Pb O
2 5 0.28081     2.76225     #Pb Cr
#3 4 0.06167    2.85440     #Ni O
3 5 0.39241     2.30825     #Ni Cr
#4 5 0.06490    2.88185     #O Cr
end
```

The FeNiCr material system for corrosion simulation can be seen in **Fig. 4.**

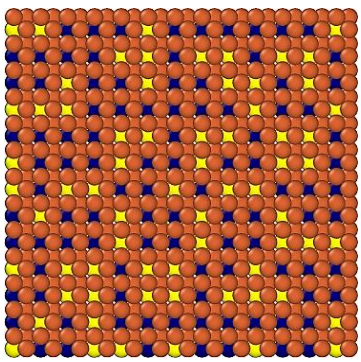


**Fig. 4.** Fe(75.40)Ni(10.57)Cr(14.04): (brown = iron, yellow = nickel, blue = nickel)

The final material for investigation is the FeNiCrTi. With a similar set-up as above, let's build the FeNiCrTi austenitic steel. Let's discuss this material in more detail later. All of the corrosion material systems are FePb, FeNiPb, FeNiCrPb and FeNiCrTiPb. All of the corrosion simulations are done at a temperature of 750 °C or 1023 K. it is possible to see the performance of each material system under liquid lead corrosion attack.

**2. 2. 2. Corrosion inhibition simulation**

The final simulation set-up is for corrosion inhibition using oxygen. Let's put oxygen with various concentrations into the liquid lead area randomly. It is possible to see the effect of oxygen injection on reducing corrosion. To put oxygen atoms randomly into the liquid lead, let's use the Lammps molecular dynamics program [22]. The lammps utility can put oxygen atoms randomly into the liquid lead by command:

```
.....
read_data xxx.data          # atomic positions of material
group iron type 1
group lead type 2
group nickel type 3
group oxygen type 4
group chrom type 5
mass 1 55.847               #Fe
set group lead type/fraction 4 0.0003 136567 # type 4 = oxygen
.....
set group lead type/fraction 4 0.0003 658829
.....
```

The list of concentrations of oxygen for simulation is shown in **Table 2** below.

From the simulations, we have to know the corrosion level of materials due to liquid lead. We are concerned about two points to analyze the corrosion: (1) observing the structure of materials after corrosion simulation and (2) understanding the diffusion coefficient of iron before and after oxygen inhibition.

**Table 2**

Composition of oxygen in the liquid lead (# lead=45006 atoms)

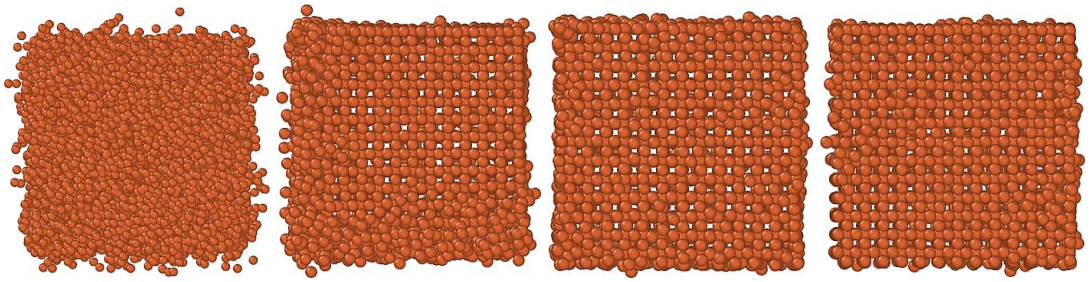
| number of oxygen | 3 | 9 | 40 | 65 | 129 | 176 | 188 | 282 | 457 |
|---|---|---|---|---|---|---|---|---|---|
| mass of oxygen | 47.997 | 143.991 | 639.96 | 1039.935 | 2063.871 | 2815.824 | 3007.812 | 4511.718 | 7311.543 |
| wt % oxygen in PbO | 0.0005 | 0.0015 | 0.0069 | 0.0112 | 0.0221 | 0.0302 | 0.0322 | 0.0484 | 0.0783 |

## 3. Results and discussion

### 3. 1. Corrosion of Fe, FeNi, FeNiCr and FeNiCrTi

**Diffusion coefficient of iron.** Let's focus on the motion (diffusion) of iron atoms of the materials under extreme high-temperature liquid lead coolant at 750 °C. Let's calculate the diffusion coefficient of iron by observing the dissolution of Fe atoms into liquid coolant. The diffusion coefficient of material can be computed by using the popular Einstein relation as we have done in previous work [10–13]. Due to our corrosion simulations being done using the Moldy program, it is easy to calculate the diffusion coefficient by calling the msd command line as described in Moldy's manual [16]. The diffusion coefficient $D(T)$ equals the slope of MSD and time $t$ divided by 6 for the 3D system. We will do discussion more detail later.

**Material compatibility**. From the simulation of FePb, FeNiPb, FeNiCrPb, and FeNiCrTiPb, it is possible to see that there is a relatively significant different compatibility of the structure among simulated materials. **Fig. 5** is the cross-section of iron/steel materials after simulation (interaction with liquid lead).



*a* *b* *c* *d*

**Fig. 5.** Compatibility of iron structures in the liquid lead:
*a* – Fe; *b* – FeNi; *c* – FeNiCr; *d* – FeNiCrTi

From **Fig. 5**, it is possible to visually see that putting other elements (Ni, Cr, Ti) into pure iron for making a steel alloy with certain composition can stabilize the structure of iron/steel more resistance to the corrosion attack of liquid lead. Adding nickel, chromium, and/or titanium for a certain concentration can increase the structural stability of material from the corrosion effect. In this study, let's only observe the AISI 316L alloy type of steel (FeNiCrTi) performance with compositions as described in **Table 3**. More detail we observe the AISI 316L steel or [Fe(75)Ni(10.57)Cr(14.05)Ti(0.40)] for corrosion study.

**Table 3**
Composition of elements in various alloy steels (# Pb = 45006 atoms)

| Materials | Pure Fe | FeNi | FeNiCr | FeNiCrTi |
|---|---|---|---|---|
| # Fe | 8788 | 6591 | 6591 | 6550 |
| wt %Fe | 100.0 | 74.1 | 75.4 | 75.0 |
| # Ni | 0 | 2197 | 879 | 879 |
| wt %Ni | 0 | 25.9 | 10.6 | 10.57 |
| # Cr | 0 | 0 | 1318 | 1318 |
| wt % Cr | 0 | 0 | 14.0 | 14.05 |
| #Ti | 0 | 0 | 0 | 41 |
| wt % Ti | 0 | 0 | 0 | 0.402 |

Now let's discuss in more detail about diffusion coefficient. The dissolution of iron in the liquid lead is important data for estimating the behavior of steels in contact with the liquid metal. The performance of materials can better seen from the diffusion coefficient. **Table 4** shows the diffusion coefficient data from our simulation work that adding elements (Ni, Cr, Ti) can reduce the diffusion of Fe atoms into the liquid lead.

From **Table 4**, there is a significant reduction in the diffusion coefficient of Fe from pure Fe, FeNi, FeNiCr, and FeNiCrTi.

**Table 4**
Diffusion coefficient of Fe in alloy steels under liquid lead, simulated at $T = 750$ °C

| Description | pure Fe | FeNi | FeNiCr | FeNiCrTi |
|---|---|---|---|---|
| diffusion $D$ ($m^2/s$) | 7.04E-08 | 5.54E-09 | 2.36E-10 | 1.59E-10 |
| compare to pure Fe | 100.00 % | 7.86 % | 0.34 % | 0.23 % |

**Fig. 6** shows the comparison of the diffusion coefficient of iron among simulated material systems: FePb, FeNiPb, FeNiCrPb, and FeNiCrTiPb. It is possible to see that the steel alloy FeNiCrTi has the most stability from corrosion under liquid lead compared to other simulated structural materials (Fe, FeNi, FeNiCr, FeNiCrTi).

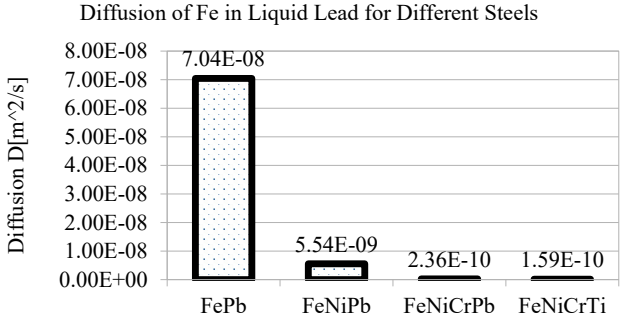



**Fig. 6.** Diffusion of iron under the liquid lead

### 3. 2. Corrosion inhibition of FeNiCrTi steel alloy

Now let's try to find a way to reduce corrosion. Since it is already concluded that the strongest FeNiCrTi steel has the most stable structure, let's limit our corrosion inhibition studies to this steel only. The above results show that the iron diffusion coefficient of FeNiCrTi in the liquid lead equals $D(1023\ \text{K}) = 1.59\times10^{-10}\ \text{m}^2/\text{s}$. This result is still big corrosion, as shown in **Fig. 4, *d***. To inhibit corrosion of structural material in liquid lead, it was popular to inject oxygen into the liquid lead coolant. The concentration of oxygen must be small enough but has an appropriate concentration to develop maximum corrosion reduction. This amount of oxygen can be predicted from simulation. In the simulation, we put oxygen atoms randomly inside the liquid lead volume. Let's prepare a PbO system with various oxygen concentrations, as shown in **Table 5**.

There are the simulations for FeNiCrTi steel or exactly Fe(75)Ni(10.57)Cr(14.05)Ti(0.40) under the influence of a liquid lead environment, together with injected oxygens. After some simulation, there are interesting results, as shown in **Table 6.**

**Table 5**

The concentration of oxygen injected into the liquid lead coolant

| # oxygen atom | 3 | 9 | 40 | 65 | 129 |
|---|---|---|---|---|---|
| mass oxygen | 47.997 | 143.991 | 639.96 | 1039.935 | 2063.871 |
| wt % oxy in liquid lead | 0.0005 | 0.0015 | 0.0069 | 0.0112 | 0.0221 |

**Table 6**

Diffusion coefficient of iron of FeNiCrTi in the liquid lead after inhibition

| wt % oxy | $D_{Fe}$ [m$^2$/s] | % corrosion |
|---|---|---|
| 0.0000 | 1.59E-10 | 100.00 |
| 0.0005 | 8.58E-11 | 54.10 |
| 0.0015 | 4.45E-11 | 28.06 |
| 0.0069 | 2.60E-11 | 16.41 |
| 0.0112 | 1.84E-11 | 11.63 |
| 0.0221 | 1.83E-11 | 11.54 |

The above **Table 6** shows significant improvement before and after the injection of oxygen. Injecting oxygen with concentration 0.0112 wt % to liquid lead coolant can reduce corrosion level (based on the diffusion of Fe) from 100 % (no oxygen) to 11.63 % only. **Fig. 7** shows values in **Table 6** in the graphical mode. The oxygen injection smaller than 0.0112 wt % still shows relatively big corrosion. However, injecting oxygen with more than 0.0112 wt % did not show a further significant improvement. From this result, it is possible to conclude that the limit for oxygen injection for effective corrosion reduction is 0.0112 wt % or $0.112\times10^{-2}$ wt % for a temperature of 750 °C. Then, if to see the structure of the materials, the structure of iron in Fe(75)Ni(10.57)Cr(14.05)Ti(0.40) is shown in **Fig. 8**.

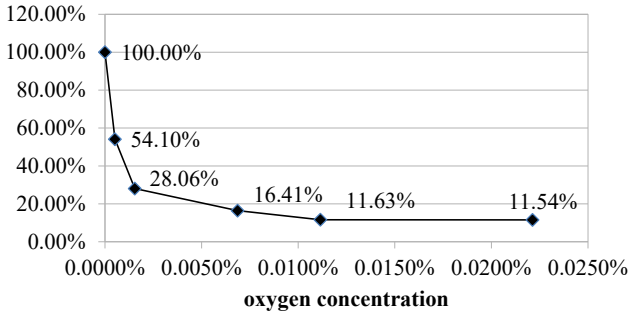



**Fig. 7.** Reduction of corrosion by injection of oxygen

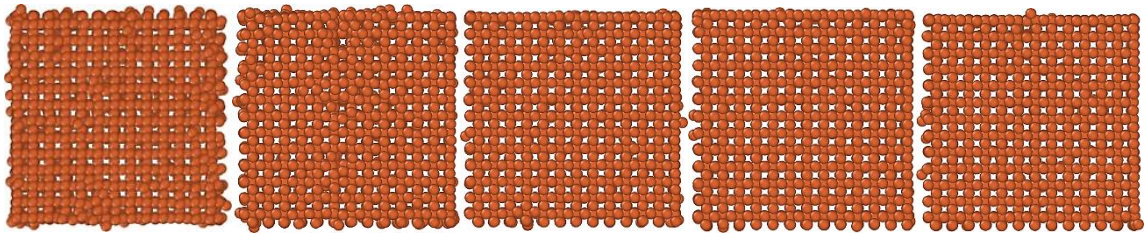



**Fig. 8.** The structure of iron in FeNiCrTi steel alloy after oxygen injection:
*a* − 0.0005 wt %; *b* – 0.0015 wt %; *c* − 0.0069 wt %; *d* − 0.0112 wt %; *e* − 0.0221 wt %

Now, let's see the available experimental results that another researcher has done. The experimental result reported that the threshold oxygen concentration associated with the onset of dissolution corrosion in 316L steel lies between $10^{-6}$ and $10^{-7}$ wt % oxygen for the specific exposure conditions at 450 °C [23].

The other research reported oxide dispersed steel (ODS) corrosion inhibition in liquid PbBi with high oxygen concentrations. At 650 °C, a high ($10^{-4}$ wt %) oxygen concentration for injection shows a good corrosion resistance [24]. It seems from those results that using a higher oxygen concentration for higher temperatures may improve the corrosion resistance of the steel.

In our current simulation result, the order of oxygen injection limit is about $10^{-2}$ wt % for a temperature of 750 °C. This relatively big difference between our result ($10^{-2}$ wt %) and experiment ($10^{-4}$ wt %) may depend on many factors. First, our simulation used the Lennard-Jones potential for describing the interaction among atoms. This potential may not be so accurate in representing steel. Second, only four atoms (FeNiCrTi) was used to represent the 316 L steel rather than more realistic multi-elements factory steel. Third, our simulation was done at a temperature of 750 °C, not 450 °C, and under liquid lead, not liquid Pb-Bi. Fourth, our simulations only used a few thousand atoms which may not be good enough to describe a realistic material system.

However, it should be noted here that the molecular dynamics simulation has shown a limited concentration of injected inhibitor for maximum corrosion reduction of materials under study. Also actually it is possible to make a comparison good among types of steels which one will show a good performance. For example, Fe(75)Ni(10.57)Cr(14.05)Ti(0.40) have shown more compatibility compared with FeNi and FeNiCr if immersed in the liquid lead. Although this method has not been able to predict accurate results, it can qualitatively predict the corrosion properties of steel in molten metal. It is possible to use it to see how the alloy steel's composition affects the material's strength against corrosion. At least it is possible to predict at what composition steel is resistant to corrosion of molten lead. Therefore the improvement of this method for accurate results is to use the interaction potential function, which is more accurate than the Lennard-Jones potential, to use a larger number of an atom to describe the material system being studied and perhaps some other improvements that can be made to model the material system better.

Our simulation work also has shown that austenitic stainless steel should also be suggested as a good material candidate for nuclear fusion reactor application. The austenitic stainless steels

are also versatile materials to be considered and applied for fast-breeder reactors. Austenitic stainless steels usually contain 15−20 % of Cr and 8−15 % of Ni as alloying elements [25]. Then due to the potential development of these austenitic steels, to obtain more comprehensive research results, it is necessary to carry out further next simulations by considering variations in concentration or composition of elements Fe, Ni, Cr, Ti, and others to find the most appropriate composition and concentration that is more resistant to corrosion of molten liquid lead at high temperatures.

## 4. Conclusions

In conclusion, the performance of several materials in liquid lead coolant have been observed that:

– adding some elements (Ni, Cr, Ti) into the pure iron crystal (to build alloy steel) seems capable to make the material more strong and structurally compact, more resistant to the corrosion attack of liquid lead;

– for specific composition of steels, from weaker to stronger and resistant to corrosion attack, we may be able to sort that: Fe ≪ FeNi < FeNiCr < FeNiCrTi. The composition of FeNiCrTi steel is Fe(75)Ni(10.57)Cr(14.05)Ti(0.40);

– the corrosion of FeNiCrTi in the liquid lead that is still high, may be effectively reduced by injecting 0.0112 wt % oxygen into liquid lead, for temperature of 750 °C.

## Conflict of interest

The authors declare that there is no conflict of interest in relation to this paper, as well as the published research results, including the financial aspects of conducting the research, obtaining and using its results, as well as any non-financial personal relationships.

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