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FeNi STEEL ALLOYS UNDER EFFECT OF MOLTEN LEAD LIQUID AT HIGH TEMPERATURE 750 ℃: A MOLECULAR DYNAMICS SIMULATION STUDY

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ABSTRACT

Materials that have superior properties are indispensable for technological applications. Steel that has strong, heat-resistant, corrosion-resistant properties is indispensable for application in the design of liquid lead metal-cooled nuclear reactors. One of the steels that need to be studied for superior properties is FeNi alloy steel. In this study, the influence of FeNi steel composition was studied using computational methods of simulating molecular dynamics. The exact composition of FeNi steel to be able to work in liquid lead reactor coolant was analyzed using the CNA (common neighbor analysis) method. Molecular dynamics simulation uses the MOLDY program while the calculation of CNA values uses the OVITO program. From the simulation results, it can be known the effectiveness of variations in Fe and Ni composition that are able to produce the most stable FeNi alloy steel from the influence of liquid lead metal corrosion.

Keyword: liquid metal corrosion, reactor coolant, liquid lead, molecular dynamics.

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1. INTRODUCTION

Molten liquid lead coolant material has been already known to have high potential applications in fast nuclear reactor design [1]. However, it is also well known that this coolant causes severe corrosion of steel (iron, nickel, chromium, etc. based alloys), especially at high-temperature conditions [1, 2-4]. Therefore, finding new high temperature resistant materials are important goal in liquid metal-cooled reactor designs. Much research has been done for these purposes, and using computational methods, the efforts can be done efficiently. Maulana *et al*. (2008) have applied the molecular dynamics (MD) method to investigate the FeNiCr steel by observing the diffusion of atoms [5].

In our previous studies (2019) we used the MOLDY molecular dynamics program developed by Prof Keith Refson to investigate the FeNiCr steel with certain composition [6, 7]. For MD simulation methods, the interatomic potential energy model is very important for accurate calculation. We have developed the new formula for the accurate calculation of Lennard-Jones parameters of different pair of atoms for metal systems [8]. We have also studied the FeNiCrTi alloy performance in molten lead liquid alloy, with certain composition [9]. In those our studied we still used the MOLDY MD program, but we did not evaluate to find the compositions variation of material. It is in this work we want to study the composition effect of Fe and Ni for FeNi steel alloy that performing the best FeNi for the used in liquid lead coolant. In this study we still use the MOLDY MD code to simulate the phenomena. Analysis of the composition variation effect on the structural stability of FeNi in liquid lead is done by the CNA (common neighbor analysis) using the OVITO program [10].

2. LITERATURE REVIEW

In MD simulation, atoms that make up the material will interact each other under specific potential energy $U(r)$ to define the force $F = -U(r)$ for a conservative system. The dynamics of atoms in some conditions then will follow Newton's law of motion $F = d\boldsymbol{p}/dt$. In our study, we will simulate the phenomena under consideration using the Moldy program. This code or program is very accurate for calculation of the properties. To represent the atomic interatomic potential of material we use the Lennard-Jones (LJ) potential (with parameter σ and ε) [11]. The LJ (6-12) can be written as following:

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

These parameters have units (for MOLDY code), σ is in Å and ε is in eV. The LJ potential is simple potential model, but we have developed the new mixing formula that may be suitable for liquid metal system [8].

3. SIMULATION METHOD

The goal of the study is to find the best composition that showing the most stable of the steel crystal structures of FeNi under molten liquid lead coolant at high temperature 750 ℃. Simulation uses the MOLDY code that need two files of input, the specification file and control file.

The control file is witten as below:

```
sys-spec-file=FeNifrac.in
title=--Moldy on liquid metal corrosion --
time-unit=1.0181e-14
lattice-start=1
const-temp=1              # Nose_Hoover Thermostat
temperature=1023          # Kelvin
const-pressure = 4        # Andersen constant pressure
pressure = 0
save-file=file.save
backup-file=file.back
dump-file=file.dump%d
begin-dump=20000
dump-level=3
dump-interval=1000
scale-options=2
nsteps = 30000
print-interval=1000
roll-interval=1000
begin-average=20000
average-interval=1000
step=0.0001
subcell=2
cutoff=8.5125  #2.5 * sigma
end
```

The specification file is written as follow (for certain composition 50%Fe-50%Ni):

```
iron 8985
1 0 0 0 55.847 0 Fe
lead 13497
2 0 0 0 207.19 0 Pb
nickel 8984
3 0 0 0 58.6934 0 Ni
end
lennard-jones
1    1    0.5193   2.3193   #Fe
2    2    0.1909   3.1888   #Pb
3    3    0.3729   2.2808   #Ni
1    2    0.31485610999312        2.75405
1    3    0.440053371763017       2.30005
2    3    0.266808189529482       2.7348
end
Lx Ly Lz 90 90 90 1 1 1  # L is dimension of supercell
Fe x y z
.....
Ni x y z
.....
Pb x y z
.....
end
```

After the simulation then the file dump (atomic trajectory in XYZ format) will read by OVITO code and using manipulation facility we can compute the CNA value of dump file to know how stable of the FeNi steel under liquid lead corrosion. Then we do many simulations with several composition variation FeNi to find the best. The more FCC % in CNA calculation, the more stable of FeNi.

4. RESULTS AND DISCUSSIONS

4.1 Composition of FeNi

To simulate the corrosion phenomena (and observing the stability of FeNi structure under extreme condition, corrosion and high temperature), all simulations was done with the same control file of MOLDY input, but different composition of FeNi. Table-1 is describing the materials.

Table-1. Composition of FeNi (in number of atom and weight %).

Metal	%Fe in FeNi	%Ni in FeNi	Pb
Pure Nickel	0	17969 (100 %)	13497
Pure Iron	17969 (100 %)	0	13497
Fe50%Ni 50%	8985 (50 %)	8984 (50%)	13497
Fe25%Ni75%	4492 (25%)	13477 (75%)	13497
Fe75%Ni25%	13477 (75%)	4492 (25%)	13497

4.2 Initial Condition of Simulated Material

Before simulation, the Fe/Ni/FeNi was prepared in the center of liquid lead, the temperature is 1023K or 750 ℃, for example is below Figure-1.

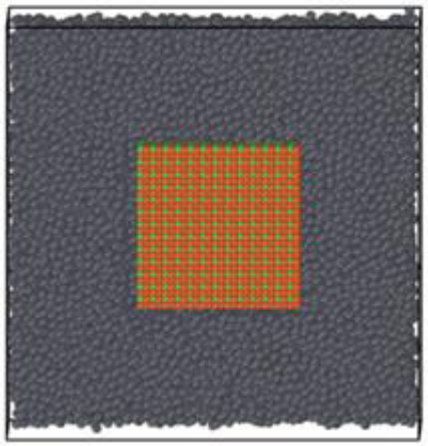
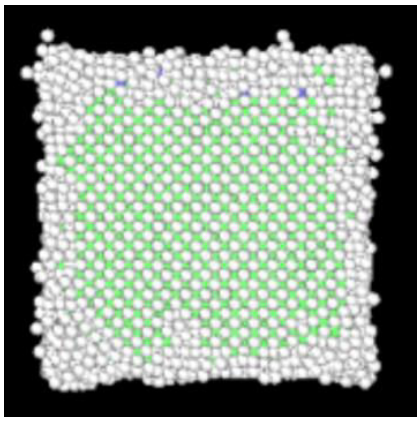


Figure-1. FeNi in liquid lead.

4.3 Nickel in Liquid Lead

After simulation the structure of pure nickel (Ni) and the CNA value is as Figure-2 below.

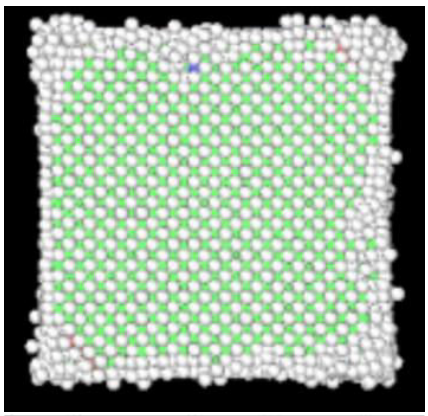


Structure	Count	Fraction	Id
Other	3775	21.0%	0
FCC	14173	78.9%	1
HCP	7	0.0%	2
BCC	14	0.1%	3
ICO	0	0.0%	4

Figure-2. Structure and CNA table value of Ni after simulation.

4.4 Pure Iron in Liquid Lead

After simulation, the structure of pure nickel (Fe) and the CNA value is shown in Figure-3 below.

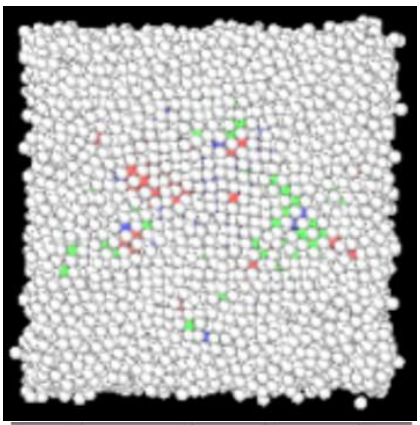


Structure	Count	Fraction	Id
Other	3366	18.7%	0
FCC	14588	81.2%	1
HCP			
BCC			
ICO	0	0.0%	4

Figure-3. Structure and CNA table value of Fe after simulation.

4.5 Fe50%Ni50% Steel Alloy in Liquid Lead

After simulation, the structure of Fe50%Ni50% and the CNA value is as Figure-4 below.

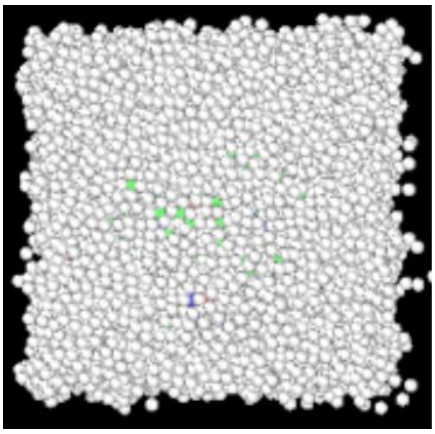


Structure	Count	Fraction	Id
Other	14348	79.8%	0
FCC	1943	10.8%	1
HCP	579	3.2%	2
BCC	1099	6.1%	3
ICO	0	0.0%	4

Figure-4. Structure and CNA table value of Fe50%Ni50% after simulation.

4.6 Fe25%Ni75% Steel Alloy in Liquid Lead

After simulation, the structure of Fe25%Ni75% and the CNA value is as Figure-5 below.

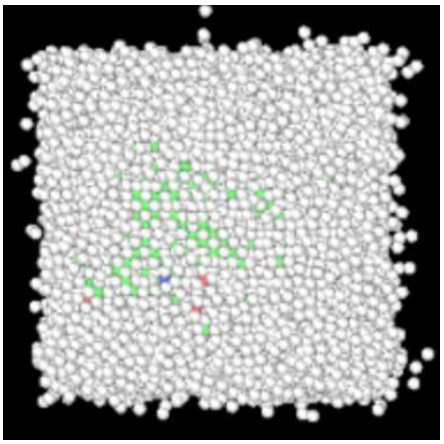


	Structure	Count	Fraction	Id
☑	Other	10302	57.3%	0
☑	FCC	7579	42.2%	1
☑	HCP	21	0.1%	2
☑	BCC	67	0.4%	3
☑	ICO	0	0.0%	4

Figure-5. Structure and CNA table value of Fe25%Ni75% after simulation.

4.7 Fe75%Ni25% Steel Alloy in Liquid Lead

After simulation, the structure of Fe75%Ni25% and the CNA value is shown in Figure-6 below.



	Structure	Count	Fraction	Id
☑	Other	9237	51.4%	0
☑	FCC	8660	48.2%	1
☑	HCP	19	0.1%	2
☑	BCC	53	0.3%	3
☑	ICO	0	0.0%	4

Figure-6. Structure and CNA table value of Fe75%Ni25% after simulation.

4.8 Discussion

From the summary table above, we get some interesting illustrations, that the composition of the atoms of a material, especially Fe and Ni-based, greatly determines the characteristics of a material. In this study, we want to see how the compactness of the structure of materials with a certain composition if the material is included in a liquid Pb environment at a temperature of 1023K. In the first case for Ni metal, it turns out that the original number of FCC structures is 100%, but after interacting with molten Pb metal for a certain time (30000 integration steps) has corroded so that the number of FCC structures becomes 78.9%.

Then in the second case for Fe metal, it turns out that the original number of FCC structures is 100%, but after interacting with liquid Pb metal for a certain time (30000 integration steps) has corroded so that the number of FCC structures becomes 81.2%.

In the third case for Fe50%Ni50% metal, it turns out that the original number of FCC structures 100%, but after interacting with liquid Pb metal for a certain time (30000 integration steps) has corroded so that the number of FCC structures becomes 10.8%.

For the fourth case for Fe25%Ni75% metal, it turns out that originally 100% FCC structure number, but after interacting with molten Pb metal for a certain time (30000 integration steps) has corroded so that the FCC structure number becomes 42.2%.

In the fifth case for Fe75%Ni25% metal, it turned out that the original number of FCC structures of 100%, but after interacting with molten Pb metal for a certain time (30000 integration steps) has corroded so that the number of FCC structures becomes 48.2%.

From the data above, we can see that the use of pure metal Fe for applications in liquid Pb is more resilient than the use of pure metal Ni which is shown by the amount of FCC Fe 81.2% > 78.% FCC Ni.

From the above data we can also conclude that the use of FeNi alloy metal for applications in liquid Pb has tough characteristics against successive corrosion from weak to stronger as follows: Fe50%Ni50%Fe50%Ni50% < Fe25%Ni75% < Fe75%Ni25%. This is consistent with the characteristics with the above pure metals, i.e. larger amounts of Fe exhibit greater toughness against liquid Pb corrosion.

5. CONCLUSIONS

In real applications, the use of Ni in combination with Fe has the aim of making composite steel stronger or others because in general (with defects) pure metals are softer than alloys. In our simulation, the pure Fe and Ni is ideal crystal with no defects for simple calculation. Therefore, the simulations in this study show that in the face of corrosion liquid Pb, Fe must be more than Ni, to make FeNi alloy steel. This can be seen from the CNA FCC grade of Fe75%Ni25% steel which is higher than Fe25%Ni75% steel.

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