Simulatian of self diffusion of iron (Fe) and Chromium (Cr) in Liquid lead by Molecular Dynamic

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Abstract— Number of rectors have become more and more from year to year, and there are currently around 800 reactors operated around the world. Fast breeder reactor then is one of the new types of reactors design, that are still being developed. Then the corrosion resistance of steels used in reactor, is one focus of today researches, due to the corrosive nature of material immersed in high temperature molter liquid metal, as Pb coolant. A strong interaction between the atoms of steels with molten metal at high temperatures causes of occurrence of diffusion processes between the steel and the cooling material. Self diffusion coefficient is a physical parameter that may be used to identify the corrosivity of steel. The choice of using the selected material than is crucial in nuclear reactors design. The corrosion simulations were run using LAMMPS molecular dynamics software. This simulation showed that adding Cr in the FeCr was placed in the center of liquid lead does not have effect for self diffusion of iron.

Keywords: Chromium, Molecular Dynamic

INTRODUCTION

Number of rectors have become more and more from year to year, and there are currently around 800 reactors operated around the world. Fast breeder reactor then is one of the new types of reactors design, that are still being developed. Then the corrosion resistance of steels used in reactor, is one focus of today researches, due to the corrosive nature of material immersed in high temperature molter liquid metal, as Lead coolant. Metal Lead liquid as a coolant in fast breeder reactor has advantages including a high melting point and good heat transfer . However, Lead liquid as a coolant fast breeder reactor is corrosive to the steel used as a coating reactor [6]. FeCr alloys selected as a coating component in the reactor because it has a good ability at high pressure and temperature, and has good resistance to corrosion.

This research will be carried out simulations with molecular dynamics methods to review the effect of adding chromium in FeCr alloys are placed in a liquid metal Lead. Molecular dynamics (MD) is a computer simulation technique by reviewing changes in the timing of groups of atoms or molecules that interact regularly [2]. Molecular dynamics method works on the principle of classical mechanics that Newton's law equation. Newton's equation of motion is written:

$$F_i = m_i \frac{\partial^2 r_i}{\partial t^2} \quad (1)$$

In classical mechanics of motion states that force is the negative of the gradient of the potential function:

$$F_i = -\nabla_i V(r_i, \dots, r_N) \quad (2)$$

The eq. (1) may be written as

$$m_i \frac{\partial^2 r_i}{\partial t^2} = -\nabla_i V(r_i, \dots, r_N) \quad (3)$$

where r is position of atom(m), m is mass of atom, and V is interaction potential of the system (Fransson and Hakansson).

Molecular dynamics simulations produce microscopic information in the form of coordinates and velocities of atoms - atoms. This research will be used LAMMPS open source program that is easy to obtain and are equipped with a manual program so easy to learn.This simulation was run using Lennard-Jones potential is modeled by two separate forces between neutral molecules and atoms. Lennard Jones potential equation can be written as a function of potential depends on the distance and energy:

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

Lennard-Jones parameters for atoms of different types modeled with a combination of Lorentz-Berthelot equation. For the parameters of the distance between the two different types of atoms that produces the equation:

$$\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j) \quad (5)$$

for energy parameters;

$$\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j} \quad (6)$$

Table 1. Lennard-Jones Potential Parameter

Pair-Interaction	σ(Å)	Ɛ (eV)
Fe-Fe	2.3193	0.4007
Cr-Cr	2.3357	0.4129
Lead –Lead	2.3275	0.1910

The mechanism of corrosion caused by the influence of diffusion that occurs between the atoms of steel coatings and atoms reactor cooling material. Self diffusion coefficient is a physical parameter that may be used to identify the corrosivity of steel. Microscopic Diffusion is defined as the displacement of atoms from the lattice to the other grating [3].

Arrhenius equation for the diffusion as the average displacement of atoms is temperature dependent written as follows:

$$D = D_0 \exp\left(\frac{-Q_d}{RT}\right) \quad (7)$$

The diffusion coefficient in computer simulations computed as the correlation function of the mean squre displacement (MSD).

$$MSD = \frac{1}{N}\sum_{i=1}^{N} \langle |r_i(t) - r_i(0)|^2 \rangle \quad (8)$$

$$D = \lim_{t\to\infty} \frac{1}{6t} MSD(t) \quad (9)$$

Where Do is the activation energy of the material, t is time is simulation, T is temperature, and R is a gas constant. Mean Square Displacement (MSD) is defined as the mean square atomic displacements in the system (Fransson and Hakansson). Diffusion coefficient values obtained by connecting the MSD against time in order to obtain the equations corresponding to the trajectory formed. Based on the above equation, the gradient produced is defined as the value of the diffusion coefficient.

This research will be reviewed at the effect of adding the element chromium FeCr alloy that was placed in the center of the liquid lead by calculating the value of the diffusion coefficient of self-diffusion of pure iron with themselves after the addition of chromium.

METHODS

The Simulation of self diffusion of iron in the FeCr alloy was placed in the center of the liquid lead. Model of FeCr alloys with 10745 atoms with a size of 48.1 x 48.1 x 48.1 A^3 that was placed in the center of the liquid lead with 45006 with a size of 122.6 x 123.8 x 125.1 A^3. Initial coordinates obtained atom, run simulations to calculate the MSD (mean square displacement) of the system. Variations addition of chromium is given at 1%, 2%, 4%, 7%, 10%, 13%, 16%, 19%, 22%, 25%, 28%, 31%, 34% 37%, 40%, 43%, 46%, 49%, and 59%, the variation is done in the form of atomic fraction (% at Cr in FeCr alloy). The system is simulated with a rise in temperature of 7000 C, 8000 C, 9000 C, C 10000, 11000 C, C 12000, 13000 C by step integration of 0.0001 ps Diffusion coefficient values obtained by connecting the MSD against time in order to obtain the equations

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corresponding to the trajectory formed. Based on the above equation, the gradient produced is defined as the value of the diffusion coefficient. The simulation results will be compared with the value of self-diffusion of pure iron are included in liquid Lead metal.

RESULTS AND DISCUSSION

In the simulation generates self diffusion coefficient values Iron in FeCr alloys are placed in liquid lead. Based on the simulation showed that the addition of Cr did not produce a linear relationship to the value of self-diffusion of iron. The lack of self-dependent diffusion of iron to the addition of Cr in the alloy FeCr has been observed previously by [4] and [5] which states that the addition of Cr in FeCr alloys have no impact on the production of atomic vacancy. However, based on chart 1. shows that the self-diffusion lowest value obtained when the concentration of Cr given as much as 22% at Cr in FeCr alloys were placed on liquid Pb metal. Difference in self-generated diffusion of the Cr concentration variations are not too large. So through this simulation known that the effect of the addition of Cr variation in FeCr alloys in molten metals Pb provides a relatively small effect on the diffusion of iron themselves.

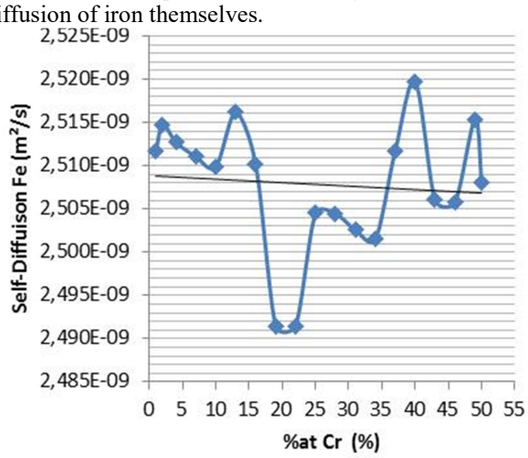

Fig. 1 Self-Diffusion Fe for chromium variation

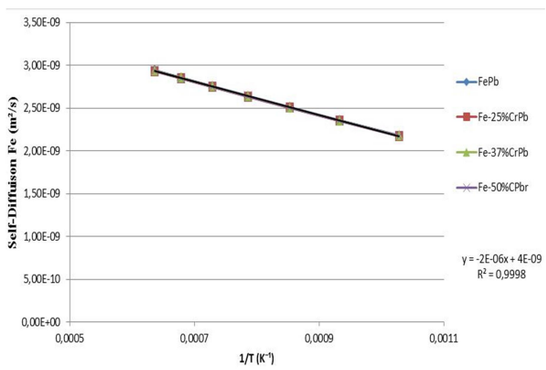

Fig. 2. Self-Diffusion Fe for Fe-Pb and FeCr-Pb

Figure 2 shows a comparison based on the self-diffusion of pure iron is placed in liquid lead metal by diffusion itself on FeCr alloy is placed in a liquid metallic lead. The simulation results show that adding Cr does not affect the self-diffusion of iron. It is shown by the graph of self diffusion of Fe in the molten metal and iron self-diffusion in the liquid metal alloy FeCr in huddle. So through this simulation shows that the addition of Cr does not affect the value of self-diffusion of iron.

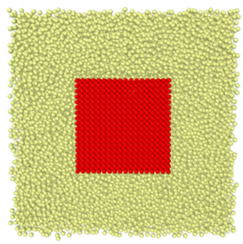

Fig. 3 Visualization of Fe in liquid lead

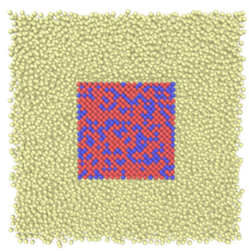

Fig. 4 Visualization of FeCr in liquid lead

We use OVITO to visualization our simulation. Based our visualization showed that adding Cr does not change the structural af atomic. Based of CNA analysis showed that strustural of atomic are same for Fe-Pb and for FeCr-Pb. This simulation never Information authors of this simulation has never been done before so it still needs reexamination to review the effect of adding Cr validation of the self diffusion of iron in the alloy FeCr placed in liquid Pb.

CONCLUSION

Based this simulation showed that adding Cr in the FeCr was placed in the center of liquid lead does not have effect for self diffusion of iron

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