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Effect of nitrogen and argon as iron corrosion inhibitors in Pb-Mg eutectic

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Effect of Nitrogen and Argon as Iron Corrosion Inhibitors in Pb-Mg Eutectic

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Abstract. The corrosion of steel due to interaction with molten metal in a nuclear reactor is an important thing to study. Liquid metal is corrosive to cladding material (steel). One solution to overcome this problem is to inject an inhibitor into the liquid metal. This study aims to compare the potential of nitrogen and argon in reducing the rate of iron corrosion on Pb-Mg eutectic using molecular dynamics methods. In this study, we use the iron to represent steel. The corrosion rate of the iron is described by the diffusion coefficient profile. A low diffusion coefficient profile indicates low iron corrosion. The results showed that nitrogen and argon had almost the same potential as iron corrosion inhibitors in Pb-Mg eutectic. The inhibitor concentration (both nitrogen and argon) was able to inhibit corrosion optimally at a concentration of 0.1798 wt% (temperature 973K). The inhibition of iron corrosion by nitrogen was 96.56% while the inhibition of iron corrosion by argon was 96.23%. If we compare the two inhibitors, it will be easier to use nitrogen, because the composition of nitrogen in the atmosphere is much higher than argon.

Keywords: nitrogen, argon, iron, Pb-Mg eutectic, molecular dynamics

INTRODUCTION

Argon is one of the most abundant noble gases in the air (about 1%) after oxygen and nitrogen [1]. Argon is the most commonly used gas in research, especially in industry because of its excellent thermal performance and lower cost efficiency than other gases [2]. Pure argon can be used as a shielding and support gas to prevent oxidation of metallic materials [3]. Sa'adah stated that argon is one of the most effective noble gases as iron corrosion inhibitor [4].

Nitrogen is one of the components that make up 78% of the air in the Earth's atmosphere [5]. In terms of corrosion resistance, nitrogen plays an important role as an alloying material for stainless steels [6]. According to Rani and Basu, nitrogen has a high level of basicity and electron density so that it can be used as a corrosion inhibitor [7]. Arkundato has conducted research on the corrosion inhibition of iron in lead-bismuth eutectic using nitrogen. He stated that nitrogen can reduce the corrosion of iron to 99.5 °C at 750 °C [8]. Both argon and nitrogen materials have advantages that can be used as iron corrosion inhibitors, so it is necessary to compare their effectiveness in inhibiting corrosion.

Corrosion is a common problem with steel and has a major impact on the cost and safety of industrial machinery. Corrosion causes structural damage and mechanical changes. So a number of studies were conducted to find an effective method of corrosion inhibition [9].

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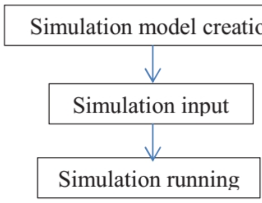
One example of a crucial corrosion problem occurs in nuclear reactor applications. Nuclear reactor technology continues to be developed to improve safety and security. One of the reactor designs is a liquid metal cooled reactor that uses materials such as lead metal [10].

At high temperatures, lead tends to damage steel components [10]. One way to overcome/reduce the occurrence of corrosion due to the interaction between steel and lead is to add lead alloy material, namely magnesium. Alekseev stated that lead magnesium alloy (PbMg) can be used as a liquid metal in nuclear reactors with concentrations of Pb (0.83%) and Mg (0.17%), with a melting point of 248 °C [11]. In 2020, Sa'adah conducted research on the corrosion of iron in lead-magnesium eutectic metals. The results obtained are iron corrosion shows a fairly high rate in the lead-magnesium eutectic [12].

Magnesium is a lightweight material and has good properties, such as easy to form, excellent mechanical properties, and can be recycled [13]. Magnesium alloys are in great demand in various industrial fields, especially the automotive industry. This is because magnesium alloys have high strength characteristics [14].

The increasing use of magnesium alloys motivates researchers and academics to apply more widely in various fields. Magnesium has a high specific heat so that magnesium will stay cold as a heat sink [15].

EXPERIMENTAL METHOD



Simulations were carried out by giving different inhibitors, namely nitrogen and argon. Both inhibitors were added alternately into liquid PbMg. The concentration variations of the inhibitors given were 0 atoms, 340 atoms (0.067 wt%), 450 atoms (0.090 wt%), 674 atoms (0.135 wt%), 906 atoms (0.1798 wt%), 1132 atoms (0.225 wt%)), and 1348 atoms (0.269 wt%).

The simulation is run in the Moldy program. The simulation data is processed to find the value of the diffusion coefficient. Based on this value, it is possible to determine the level of inhibition of iron corrosion due to the administration of argon or nitrogen inhibitors.

Equations to determine the diffusion coefficient,

$$D = \lim_{t \to \infty} MSD \ / \ 6t \tag{1}$$

where,

$$MSD = \left\langle \left| \vec{R}(t) - \vec{R}(0) \right|^2 \right\rangle \tag{2}$$

MSD is Mean Square Displacement, t is simulation time (ps), and $\vec{R}$ is atomic position.

While the temperature dependent diffusion coefficient is calculated using the Arrhenius equation,

$$D(T) = D_0 \cdot e^{\left(\frac{-A}{\Re T}\right)} \tag{3}$$

A is activation energy (J/mol), $\Re$ is universal gas constant, and T is temperature (K).

In addition, to see the appearance of the corrosion reduction results between argon and nitrogen, it can also be done by calculating the amount of remaining iron crystal structure using the Ovito program.

RESULTS AND DISCUSSION

The simulation in this study was carried out in two stages, that is the simulation of iron in eutectic Pb-Mg before being given the inhibitor and the simulation of iron in eutectic Pb-Mg after being given the inhibitor. After simulating the MSD data obtained, then using equations (1) and (3), we can calculate the value of the diffusion coefficient. The diffusion coefficient value of iron in eutectic Pb-Mg before being given the inhibitor is 1.2483 x 10^{-9} m^2/s at a temperature of 973K.

In this study, the results of running simulations were obtained that illustrated the diffusion coefficient profile of iron in Pb-Mg eutectic given nitrogen and argon inhibitors.

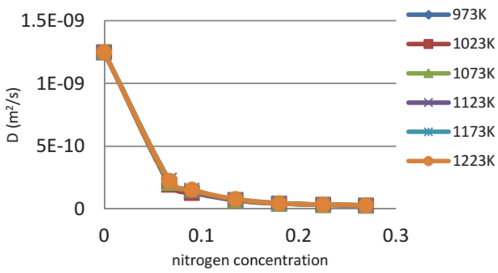


FIGURE 1a Diffusion coefficient profile of iron in Pb-Mg eutectic with nitrogen variation.

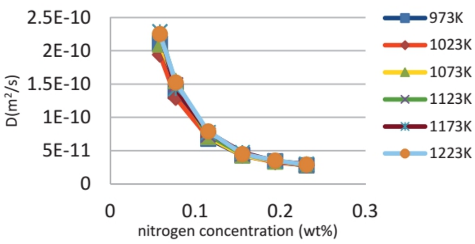


FIGURE 1b Zoom from graph 1a for nitrogen concentration greater than 0.067wt%.

Figure 1a dan 1b is a profile of the diffusion coefficient of iron in Pb-Mg eutectic given variations in nitrogen concentration with temperature variations. Figure 1a shows that nitrogen with a concentration of 0.067wt% - 0.269wt% can reduce the diffusion coefficient value from the initial order of 10^{-9} to 10^{-11}. Figure 1b is a diffusion coefficient profile with a nitrogen concentration of 0.067wt% - 0.269wt%. The diffusion coefficient curves for various temperatures show the same trend curve. The greater the amount of nitrogen concentration given, the lower the diffusion coefficient value. At a nitrogen concentration of 0.1798 wt% - 0.269 wt%, the curves seem to coincide in one line. This means that the diffusion coefficient is the same for various temperatures at that concentration.

Figure 2 is a diffusion coefficient profile of iron in Pb-Mg eutectic given variations in nitrogen concentration with temperature variations. Figure 2a shows the diffusion coefficient value before being given the argon inhibitor is 1.2483 x 10^{-9} m^2/s. After being given argon with a concentration of 0.067wt%, the diffusion coefficient increased. However, after being given several variations in the concentration of argon, the diffusion coefficient began to decline. Figure 2b shows the diffusion coefficient profile of iron with an argon concentration of 0.067wt% - 0.269wt%. The diffusion coefficient values at various temperatures show almost the same trend but the range of diffusion coefficient values is rather far. The lowest diffusion coefficient value is given a concentration of 0.1798 wt% at a temperature of 973K - 1023K. Whereas at temperatures of 1073K and 1223K the lowest diffusion coefficient values were given

0.135 wt% argon concentration. However, at temperatures of 1123K - 1173K the lowest diffusion coefficient value was given 0.1798 wt% argon concentration.

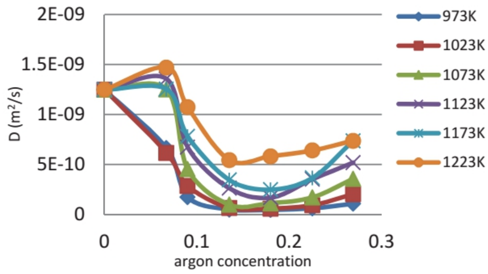


FIGURE 2a Diffusion coefficient profile of iron in Eutectic Pb-Mg with argon variation.

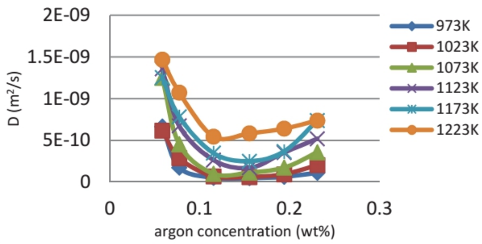


FIGURE 2b Zoom of graph 2a for argon concentration greater than 0.067wt%.

In general, the optimal concentration of argon in inhibiting iron corrosion in Pb-Mg eutectic when viewed from the average value of the lowest diffusion coefficient for various temperatures is at a concentration of 0.1798 wt%. The low diffusion coefficient indicates that the iron corrosion in Pb-Mg eutectic is also small. So the 0.1798 wt% argon concentration was able to optimally suppress the iron corrosion rate in Pb-Mg eutectic.

Figures 1 and 2 depict the different diffusion coefficient profiles. To compare the performance of the two inhibitors, it is necessary to make curve fittings by taking the lowest diffusion coefficient data at a temperature of 973K (figure 3).

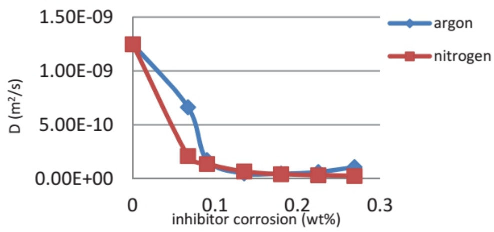


FIGURE 3a Comparison of the diffusion coefficient of iron in Pb-Mg eutectic with nitrogen and argon content at a temperature of 973K.

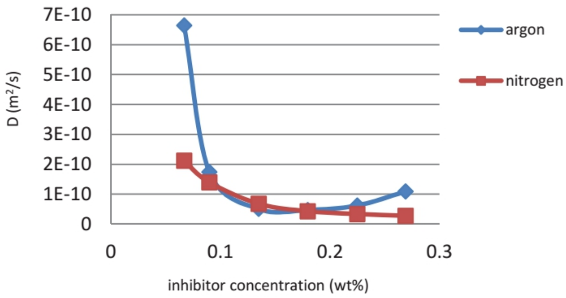
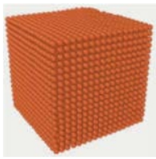


FIGURE 3b zoom from graph 3a for inhibitor concentration greater than 0.067wt%.

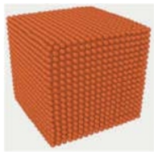
Figure 3 is the fitting of the iron diffusion coefficient curve before being given an inhibitor (Figure 3a) and the diffusion coefficient of iron after being given an inhibitor with a concentration of 0.067wt% - 0.269wt% (Figure 3b) at a temperature of 973K. In this figure, it can be seen that at concentration 0.1798 wt% the diffusion coefficient curve of iron using nitrogen and argon inhibitors is at the same point. The diffusion coefficient of iron using a nitrogen inhibitor at concentration 0.1798 wt% is 4.298 x 10^{-11} m^2/s, while the diffusion coefficient for iron using an argon inhibitor at concentration 0.1798 wt% is 4.705 x 10^{-11} m^2/s. To see the crystal structure of the iron at the same point, it can be seen in figure 4.

Figure 4a is a visualization of the crystal structure of the iron before being given the inhibitor. The image shows the occurrence of iron corrosion as seen from random crystal structure changes on the iron surface. Figures 4b and 4c are visualizations of the crystal structure of iron after being given 0.1798wt% nitrogen and argon inhibitor. Both figures show that the inhibitor is very influential in reducing iron corrosion. This is evidenced by the shape of the iron crystal structure which is close to the perfect BCC crystal structure. To find out more details about the number of atoms whose structure can be maintained, see table 2.

(a) iron corrosion before adding inhibitor



(b) using nitrogen inhibitor 0.1798 wt%



(c) using argon inhibitor 0.1798 wt%

FIGURE 4 Visualization of the crystal structure of iron in Pb-Mg eutectic with different inhibitor content at a temperature of 973K.

TABLE 1. Comparison Of The Crystal Structure Of Iron With Nitrogen And Argon Inhibitors

Inhibitor	**Iron crystal structure**	
	BCC	**Other**
Nitrogen	7470 atom (69.5%)	3275 atom (30.5%)
Argon	7469 atom (69.5%)	3280 atom (30.5%)

Table 1 shows the number of crystalline structures of iron that can be maintained by nitrogen and argon inhibitors 0.1798wt% at temperature 973K. When viewed from the percentage of atoms, the structure of the iron crystal in the form of BCC, either given a nitrogen inhibitor or argon, shows the same number. But if it is viewed from the number of atoms, the crystal structure of BCC iron which is given a nitrogen inhibitor has more atoms than the crystal structure of BCC iron which is given argon.

TABLE 2. Reduction of Iron Corrosion with 0.1798wt% Inhibitor Concentration at 973K Temperature

Inhibitor	$D_{initial}$ (m^2/s)	$D_{the\ best}$ (m^2/s)	Reduction (%)
Nitrogen	1.248E-09	4.298E-11	96.56
Argon	1.248E-09	4.705E-11	96.23

Table 2 shows that nitrogen can inhibit iron corrosion 96.56% while argon can inhibit iron corrosion 96.23%. D initial is the diffusion coefficient value of iron in eutectic Pb-Mg before being given the inhibitor. The best is the diffusion coefficient value of iron in eutectic Pb-Mg after being given an inhibitor. Thus it can be assumed that nitrogen has more potential to inhibit iron corrosion in liquid metal Pb-Mg. This assumption is also based on the amount of inhibitor material available in nature. According to the data in the encyclopedia [16] states that nitrogen in nature has the greatest amount compared to argon.

CONCLUSION

In this study, nitrogen and argon have good potential in inhibiting iron corrosion in Pb-Mg eutectic. For nitrogen inhibitors, at a temperature of 973K the greater the concentration is given, the less the diffusion coefficient value of iron in Pb-Mg eutectic. As for the argon inhibitor, at a temperature of 973K, the optimal amount of argon concentration inhibits iron corrosion in Pb-Mg eutectic at a concentration of 0.1798 wt%. If the two inhibitors are compared, the inhibitor concentration, both nitrogen, and argon, can be assumed to be able to inhibit corrosion optimally at a concentration of 0.1798 wt% (temperature 973K).

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