

Density of Liquid Lead as Function of Temperature and Pressure Based on the Molecular Dynamics Method

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Abstract. Simulation research has been carried out to obtain the formula for mass density of liquid lead as a function of temperature and pressure. The simulation method used is the molecular dynamics method. The potential energy used in the simulation is the Morse potential. From the simulation, it is found that the relationship between the mass density of liquid lead and temperature and pressure can be expressed in the equation $\rho_{Pb} = 11233 - 0,9217 \times T$ for pressure 1 – 5 atm and $\rho_{Pb} = 11233 - 0,9213 \times T$ for pressure 7 atm in units kg/m^3 .

Keywords: Liquid Lead, Mass Density, Temperature, Pressure, Molecular Dynamics.

Introduction

Currently, nuclear power plants have become one of the alternative energy sources which are becoming an interesting choice of many countries. If developed countries have long used nuclear energy to support their heavy industries, developing countries think about the use of this energy in a recent time. The nuclear reactor basically produces heat energy from the process of nuclear fission. The subsequent use in the form of conversion to electricity in large quantities is one of the attractions for the development of this nuclear energy, besides there may concerns for utilization in the field of weaponry.

The development of nuclear reactors for welfare today generally still relies on the design of thermal reactors. There are still many thermal reactors operating in this world. Unfortunately, many thermal reactors are still legacy of old designs. Since the Chernobyl nuclear reactor accident in Ukraine in the past, a safer new concept reactor design is constantly being considered. For this reason currently developing IV generation nuclear reactors. Some of the advantages of this generation IV reactor design are the inherent safety concept.

Liquid metal-cooled fast nuclear reactors, for example liquid lead, are reactor concepts and designs that apply the safety concept inherent in the design so that if there is a potentially catastrophic anomaly in the reactor, the reactor system can automatically shut down the operation of the nuclear reactor without the need for any process of manual shutdown.

More specifically, the liquid lead metal cooled fast nuclear reactor is one of the promising reactor concepts apart from applying the inherent safety concept it is also capable of being made in a modular form and producing high power energy [1].



Liquid lead metal and its alloys with other metals such as bismuth are currently promising candidate materials for cooling fast nuclear reactors [2]. There are many advantages compared to cooling water in a slow neutron nuclear reactor. One of them is that it has a high boiling point and has a large thermal conductivity, making it very suitable for cooling in fast reactor designs.

For this reason, in order for the design of a fast nuclear reactor to be made properly, complete nuclear data, for example, information on mass density, is required. Because in the reactor two factors that are very important to note are temperature and pressure, this mass density needs to be known as a function of temperature and pressure.

In this study, therefore, we want to know the density formula as a function of temperature and pressure. To obtain this, the molecular dynamics method will be used so that a lot of data can be obtained for various temperatures and pressures.

Theory

Molecular dynamics methods in general can be used to predict the physical properties of materials such as melting point, heat conductivity, enthalpy, diffusion coefficient, and so on, including predicting density as a function of temperature. What matters is whether we have sufficient potential energy data to describe the interactions between the atoms of the material system. Arkundato *et al* has used the molecular dynamics methods to investigate liquid lead coolant [3-4]. In this research, we will use the Morse potential.

In the molecular dynamics method, the Newton motion equation is solved to get the trajectories of all the atoms that make up the material. The relationship between Newton's equations of motion and potential is as follows

$$F = m \, d^2 r / dt^2 \quad (1)$$

$$F = - \, dV/dr \quad (2)$$

where F is the interacting force of particles, r position vector of a particle, V is potential energy of interacting particles. The Morse potential for this simulation has a form of [5].

$$V(r) = D_e (1 - e^{-a(r-r_e)})^2 \quad (3)$$

where r_e is the equilibrium bond distance from the atom, D_e is the bonding energy balance of an atom and a is a parameter,

$$a = \sqrt{\frac{k_e}{2D_e}} \quad (4)$$

Girifalco dan Weizer (1958) has made table of Morse potential parameters as below [6].

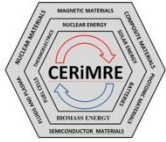


Table 1. Morse potential parameters of some cubic metals [5]

Metal	αa_0	B	$L(\text{ev}) \times 10^{-22}$	$a=A^{-1}$	$r_0=A$	$D(\text{ev})$
Pb	2.921	83.02	7.073	1.1836	3.733	0.23480
Ag	2.788	71.17	10.012	1.3690	3.115	0.33230
Ni	2.500	51.78	12.667	1.4199	2.780	0.42050
Cu	2.450	2.450	49.11	10.330	1.3588	0.34290
Al	2.347	4417	8.144	1.1646	3.253	0.27030
Ca	2.238	39.63	4.888	0.80535	4.569	0.16230
Sr	2.238	39.63	4.557	0.73776	4.988	0.15130
W	2.225	72.19	29.843	1.4116	3.032	0.9906
Cr	2.260	75.92	13.297	1.5721	2.754	0.4414
Fe	1.988	51.97	12.573	1.3885	2.845	0.4174

In our work we will use Morse potential parameter from Girifalco data. Furthermore, based on the trajectory of the atoms of the material as a solution of Newton's equations of motion then using statistical mechanics concepts and theories it can be predicted any physical quantities that we want to know. This physical quantities can be calculated easily when we use the Lammmps molecular dynamics software [6] that also we used in this research (<https://lammmps.sandia.gov/>).

Method

The purpose of this study was to find the mass density relation of liquid lead as a function of temperature and pressure. Physical variables mass density, pressure, temperature were simulated with Lammmps software. The procedure for obtaining the relationship between the three variables is carried out according to the following steps:

1. Create a script file that contains data on the position of lead atoms, mass, number of atoms, pressure, temperature, number of integration steps, compute command, etc. Table 2 is a summary of input parameters.

Table 3. Input parameters for Lammmps simulation

Variable	Value
Mass of Pb	207.2
Lattice constant	4.950 Å
Temperatures	323K, 423K, 523K, 623K, 723K, 823K, 923K, 1023K
D	0.2648 ev
r_0	3.520 A
a	1.3036 A ⁻¹
pressure	1 atm, 5 atm, 7 atm

2. Do simulation for different temperature and pressure
3. Make analysis and conclusion
4. Determine mass density as a function of temperature and pressure

Results

From lead simulation results for different temperatures and pressures then we can calculate the density as Table 4.

Table 4. Density of liquid lead at various temperatures and pressures

Temperature (K)	Mass density (kg/m ³)		
	pressure 1 atm	pressure 5 atm	pressure 7 atm
323	10918.59013	10918.71963	10918.78437
423	10839.89903	10840.03266	10840.09959
523	10758.77752	10758.90916	10758.97953
623	10673.75396	10674.02894	10674.10180
723	10582.58427	10582.73939	10582.81616
823	10479.97194	10480.13611	10481.66200
923	10356.97857	10357.16451	10357.58981
1023	10189.90371	10190.05928	10190.47230

From Table 4 we can determine the mass density as a function of temperature and pressure using linear regression method,

For pressure 1 atm:

$$\rho_{Pb} = 11233 - 0,9217 \times T \quad [1 \text{ atm}] \quad [5 \text{ atm}] \quad (5)$$

Equation (5) also applies for pressure 5 atm. For pressure 7 atm there is a little different, i.e.,

$$\rho_{Pb} = 11233 - 0,9213 \times T \quad [7 \text{ atm}] \quad (6)$$

Figure 1 shows the mass density of liquid lead at 1 atm as a result of molecular dynamics simulation.

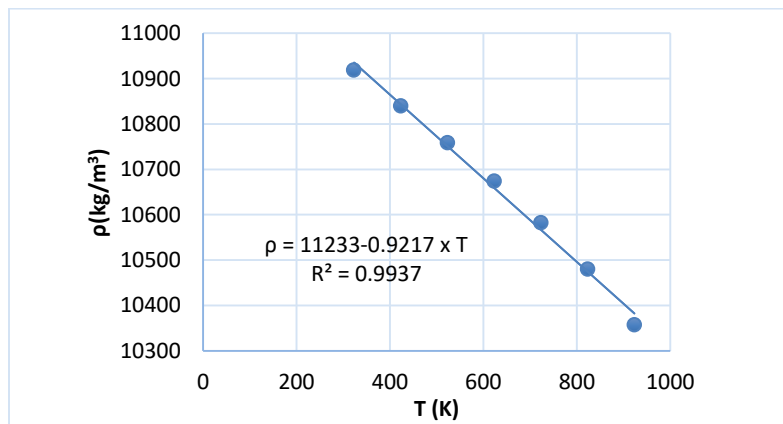


Figure 1. Mass density of liquid lead at 1 atm



Let's we compare our simulation result and a reference [7]. Sobelov states that the formulation value for the density of liquid lead at a pressure of 1 atm is:

$$\rho_{Pb} = 11441 - 1,2795 \times T \text{ [1 atm]} \quad (7)$$

We can check the discrepancy between simulation and reference as shown in Table 5.

Table 5. Comparison the mass density by simulation and reference

Temperature (K)	Mass density (kg/m ³) (simulation)	Mass density (kg/m ³) (Sobelov, 2011)	discrepancy (%)
323	10935,2909	10997,7215	0,57%
423	10843,1209	10869,7715	0,25%
523	10750,9509	10741,8215	0,08%
623	10658,7809	10613,8715	0,42%
723	10566,6109	10485,9215	0,77%
823	10474,4409	10357,9715	1,12%
923	10382,2709	10230,0215	1,49%

From Table 5 we can conclude that our simulation results are pretty good when compared to references. In our simulation we have used 500,000 atoms of Pb created by 50 x 50 x 50 boxes of unit cells in FCC crystal structure. Then this also describes that the Morse potential and its parameters is good to formulate the interaction among metallic atoms of lead.

Conclusions

The simulation results are pretty good when compared to references. The simulation method used is the molecular dynamics method. The potential energy used in the simulation is the Morse potential. In our simulation we have used 500,000 atoms of Pb created by 50 x 50 x 50 boxes of unit cells in FCC crystal structure. Then this also describes that the Morse potential and its parameters is good to formulate the interaction among metallic atoms of lead. From the simulation, it is found that the relationship between the mass density of liquid lead and temperature and pressure can be expressed in the equation $\rho_{Pb} = 11233 - 0,9217 \times T$ for pressure 1 – 5 atm and $\rho_{Pb} = 11233 - 0,9213 \times T$ for pressure 7 atm in units kg/m³.

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