Parameters (σ, ε) of Lennard-Jones for Fe, Ni, Pb for Potential and Cr based on Melting Point Values Using the Molecular Dynamics Method of the Lammps Program

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Parameters (σ, ε) of Lennard-Jones for Fe, Ni, Pb for Potential and Cr based on Melting Point Values Using the Molecular Dynamics Method of the Lammps Program

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Abstrak. Lennard-Jones potential is the potential energy of the bond interaction between two atoms or free molecules based on the distance between them. Molecular dynamics simulations can be used to calculate various physical properties of materials based on specific interaction potentials. One of the physical properties of a material is its melting point. This research was conducted to find the potential parameter values of Lennard-Jones metal Fe, Pb, Ni and Cr based on the melting point value of the material using the LAMMPS program. In this study the normalization of potential parameters is done by comparing the results of the simulation melting point with the experimental melting point. This research produces a Lennard-Jones potential parameter value which yields a melting point value that has a relatively small description.

1. Introduction

One model of potential energy between two atoms or molecules is the Lennard-Jones potential. This potential energy model is considered the simplest, which was originally applied as an argon gas model, but has good accuracy for calculating the simulation results. This potential model can be formulated as follows [1]:

$$U(R_{ij}) = k\varepsilon\left[\left(\frac{\sigma}{R_{ij}}\right)^{n} - \left(\frac{\sigma}{R_{ij}}\right)^{m}\right] \quad (1)$$

n and *m* are selected positive integers where *n*> *m*

$$k = \frac{n}{n-m}\left(\frac{n}{m}\right)^{m/(n-m)} \quad (2)$$

i and *j* are the index of the molecule $R_{ij} \equiv |R_i - R_j|$ or the distance between molecules *i* and *j*. σ is the distance parameter and ε is the parameter expressing the strength of the interaction. In general, the values of *n* and *m* are *n* = 12 and *m* = 6, so the equation for the Lennard-Jones potential can be written as follows:

$$U(R_{ij}) = k\varepsilon\left[\left(\frac{\sigma}{R_{ij}}\right)^{12} - \left(\frac{\sigma}{R_{ij}}\right)^{6}\right] \quad (3)$$

The intermolecular force on the Lennard-Jones potential can be written as follows:

$$F(R_{ij}) = -\frac{d}{dr}U(R_{ij}) = 24\varepsilon\left[\left(\frac{\sigma}{R_{ij}}\right)^{13} - \left(\frac{\sigma}{R_{ij}}\right)^{7}\right] \quad (4)$$

A positive force indicates a repulsive force and a negative force indicates an attraction. This model illustrates the existence of a repulsive force with a term $\left(\frac{\sigma}{R_{ij}}\right)^{13}$ that dominates at close range and an attractive force with a term $\left(\frac{\sigma}{R_{ij}}\right)^{7}$ that dominates the distance.

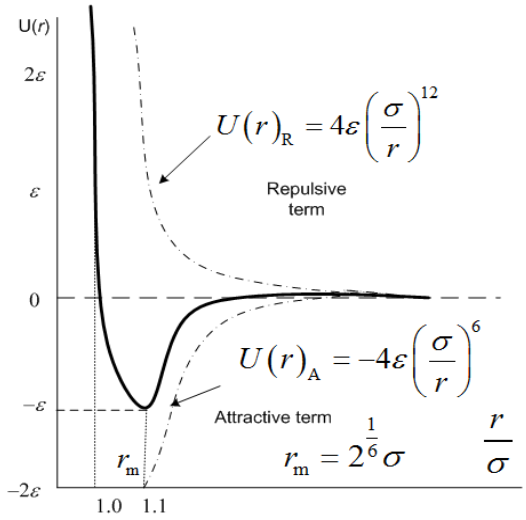


Figure 1. Potential Lennard-Jones [2]

Figure 1 shows the Lennard-Jones potential function curve. At very close distances between atoms, they will repel each other according to Pauli's principle. When located at a considerable distance will appear interactions of attraction between atoms that are influenced by Van der Waals forces due to the appearance of dipole-dipole interactions [3].

The Lennard-Jones potential has two parameters namely σ and ε and the molecular dynamics simulation is used to calculate various physical properties of materials. One physical property of a material is its melting point value. The melting point of a solid is a temperature at which an equilibrium occurs between the solid phase and the liquid phase (at one atmospheric pressure) [4]. In principle, a substance can melt because the bonds between molecules begin to weaken, where the weakening of bonds between molecules occurs at different temperatures depending on the strength of these bonds, the stronger the bond, the higher the heat needed.

The molecular dynamics method is one method that can be used to predict the physical properties of materials both mechanical, thermal and chemical. This method works using Newton's law [5-10]. The molecular dynamics method is used to see the physical properties of materials through the movement of atoms resulting from interactions using interatomic potential [11]. Realization of molecular dynamics simulations generally use a computer program. The program used for example is LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). In fact, there are many

interatomic potentials that describe interactions between material atoms. One of the famous ones is Lennard-Jones. In molecular dynamics simulations the first step that must be done is to determine the initial conditions of the material system. The very regular and periodic arrangement of atoms or molecules is called a crystal. Whereas atoms or molecules that make up crystals that are located very regularly are called lattices [12].

In this study (the objective) will be calculated the melting point of the material using molecular dynamics simulations with Lennard-Jones potential. The material studied was metal Fe, Pb, Ni and Cr. The molecular dynamics program used in this study is the LAMMPS program [13]. The LAMMPS program is designed to simulate many atoms and molecules on a small or very large scale, both done with one or multiple processors.

What's important about this research is that the melting point calculation is done by first ensuring the best value of the potential parameters (σ) and (ε) through comparative experiments. So, in this study in addition to getting the melting point value of the material also obtained the appropriate parameter values for the material (σ) and (ε) if the simulation used uses Lammps. This is the "state of the art" of this research.

2. Method

In this study to calculate the melting point value of the first step material by normalizing the Lennard-Jones potential parameters in the form of sigma (σ) and epsilon (ε) values. The normalization process of sigma and epsilon is done through the interpretation of the phase change curve from solid to liquid. Values of σ and ε in the literature will produce a melting point (TL) that is less suitable to the experiment when it is simulated using the LAMMPS application.

In this study, simulations for certain σ and ε are run, namely by changing the values of σ and ε until a simulated melting point value is obtained which has a small discrepancy by making a graph between potential energy (Ep) and temperature (T) to determine the melting point value (TL). The value (TL) of the simulation is compared with the value (TL) of the experiment, if the value of the discrepancy obtained from the simulation results is ≥5 %, then improvements should be made to the values of σ and ε, to produce a discrepancy value of ≤ 5 %.

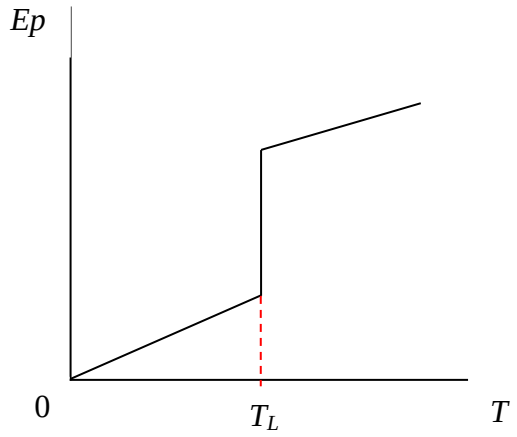


Figure 2. Graph of phase change of substances

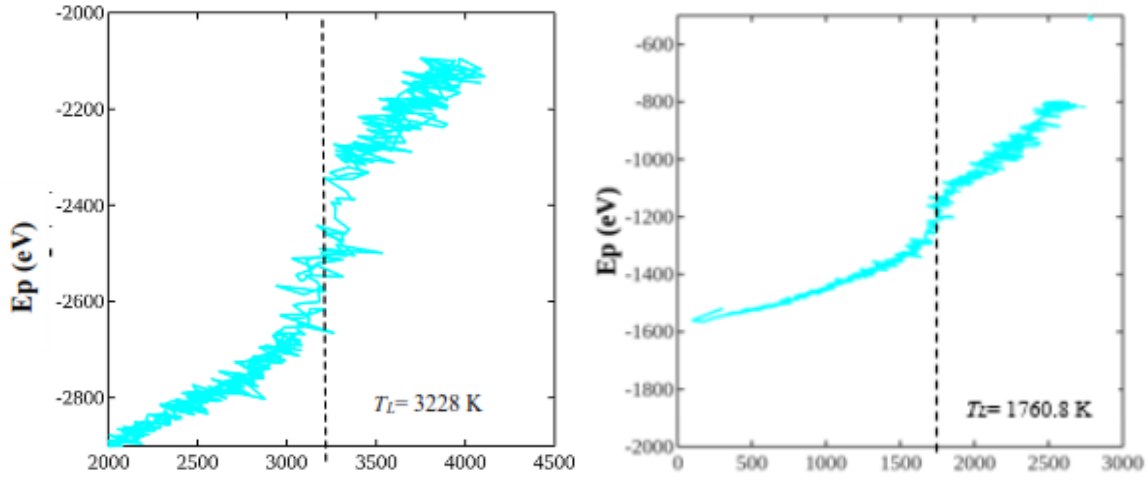
Figure 2. is a graph of phase change in the form of a relationship between temperature (T) for the horizontal axis and potential energy (Ep) for vertical axis. The graph of the changes in phase changes was created using the Octave program [14]. Octave is a program used to analyze numerical data. Calculation of the potential energy value (Ep) itself has been done by the LAMMPS program automatically.

3. Results and Discussion

Analysis of the results of the study is based on the simulation output according to the input already written in the control file. This simulation is carried out to obtain data on the melting point value of the material according to the Lennard-Jones potential parameter values, which are the sigma (σ) and epsilon (ε) values which are then compared with the experimental melting point values.

In this study the simulation output data in the form of temperature and potential energy where both graph plots will be made. The graph is the relationship between temperature (for the horizontal axis) and potential energy (for the vertical axis) so that the melting point values for each material can be determined. The melting point value is based on the graph when the temperature value remains, but the potential energy value will increase drastically.

Fe metal has initial parameters in accordance with the reference that is equal to 0.4007 eV (ε) and 2.3193 Å (σ). The melting point value generated during the simulation using the initial input of the Lennard-Jones Fe potential parameter obtained a melting point value of T_L = 3228 K and has a discrepancy of 43.89 %. Figure 3 also shows a graph of the simulation output after normalizing the Lennard-Jones potential parameters. In this study, after normalizing the Lennard-Jones potential parameter values, the best Lennard-Jones potential parameter values are obtained for Fe σ = 2.4193 Å and ε = 0.2007 eV. These parameters produce a melting point value of T_L = 1760.8 K which occurs in step 39500 with a discrepancy of 2.85 %



(a) (b)

Figure 3. Graph of metal phase changes Fe (a) before normalization and (b) after normalization of Lennard-Jones potential parameter values using LAMMPS

Ni metal has experimental Lennard-Jones potential parameters of 0.3729 eV (ε) and 2.2808 Å (σ). The simulation results from the initial parameters shown in Figure 4 (a) obtained the melting point value of T_L = 3330.9 K with a discrepancy of 48.12 %, so it is necessary to normalize the value of the Lennard-Jones potential parameter in order to obtain a good melting point value that has very small discrepancy value. Figure 4 (b) after normalizing the Lennard-Jones potential parameter values for Ni metals, the best parameters are obtained σ = 1.5808 eV and ε = 0.1729 Å. These parameters produce a melting point value of T_L = 1726.8 K with a 0.07 % discrepancy.

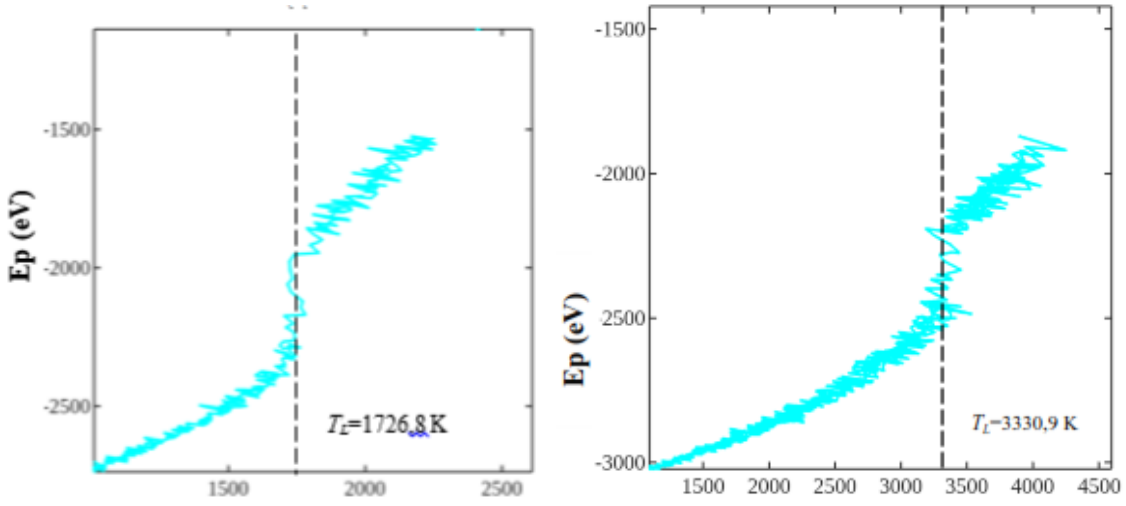


Figure 4. Graph of Ni metal phase changes (a) before normalization and (b) after normalization of Lennard-Jones potential parameter values using LAMMPS

The value of the Lennard-Jones Pb potential parameter is 0.1910 eV (ε) and 3.1888 Å (σ). Figure 5 (a) below, where the graph shows the results of the simulation output of the Lennard-Jones Pb potential parameters before normalization results in a melting point value of T_L = 1973.8 K with a discrepancy value of 69.57 %. After doing the normalization, the best parameters obtained are σ = 3.6888 eV and ε = 0.0610 Å which results in a melting point value of T_L = 598.7 K with a 0.32 % discrepancy, shown in Figure 5 (b).

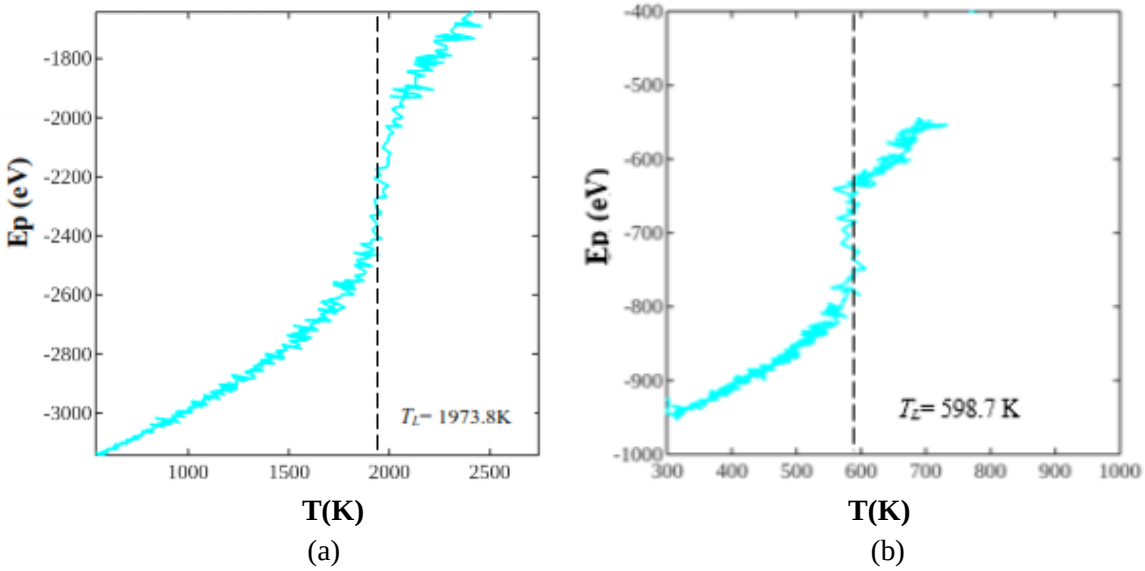


Figure 5. Graph of Pb metal phase change (a) before normalization and (b) after normalization of Lennard-Jones potential parameter values using LAMMPS

Lennard-Jones Cr potential parameter values are 0.67322 eV (ε) and 2.2813 Å (σ). The results of simulation output when using the initial input of the Lennard-Jones Cr potential parameter obtained the melting point value of T_L = 1631.9 K with a discrepancy value of 33.58 %. Figure 6 (b) shows a graph of the simulation output after normalizing the Lennard-Jones potential parameters. After normalizing the Lennard-Jones potential parameter values in Cr metal, the best parameters are obtained σ = 2.7813 eV and ε = 0.24322 Å. These parameters produce a melting point value of T_L = 2183.7 K with a discrepancy of 0.17 %.

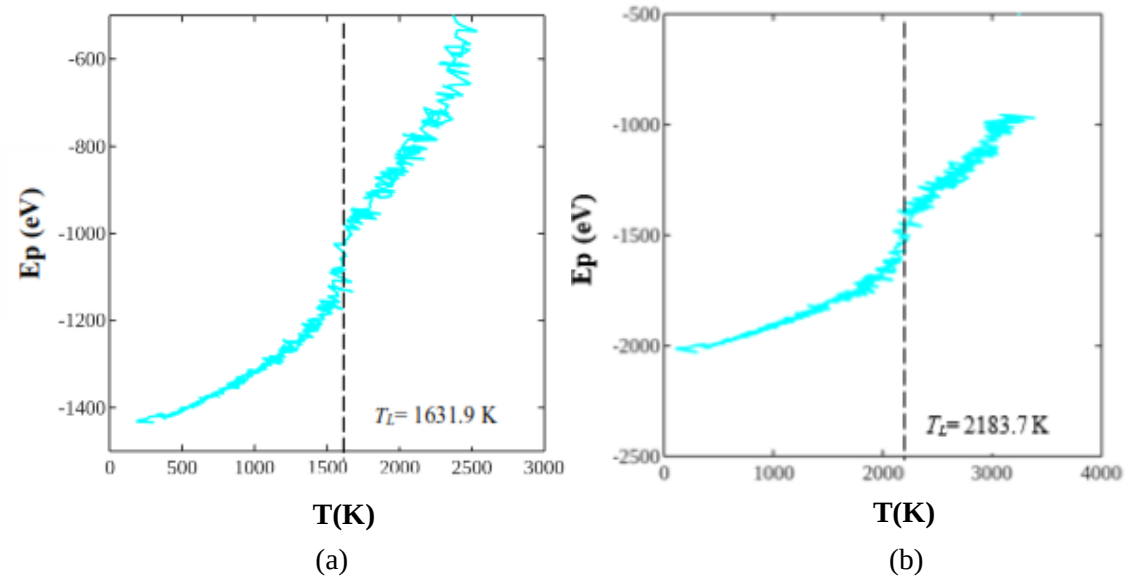


Figure 6. Graphs of metal phase changes Cr (a) before normalization and (b) after normalization of Lennard-Jones potential parameter values using LAMMPS

4. Conclusion

The conclusion from the study of the potential parameters of the Lennard-Jones metals Fe, Ni, Pb and Cr based on the melting point value using the molecular dynamics method of the LAMMPS program are:

1. Based on the molecular dynamics method the melting point value of Fe, Ni, Pb and Cr metal is the value of Fe melting point obtained by T_L = 3228 K with a discrepancy of 43.89 %, Ni for T_L = 3330.9 K with a discrepancy value of 48, 12 %, Pb of T_L = 1973.8 K with a discrepancy value of 69.57 % and for Cr of T_L = 1631.9 K with a discrepancy value of 33.58 %.
2. The value of the Lennard-Jones potential parameters that have been normalized using the LAMMPS program obtained values σ = 2.4193 Å and ε = 0.2007 eV which results in a material melting point value of T_L = 1760.8 K with a discrepancy of 2.85 %, Ni metals obtained the value of σ = 1.5808 Å and ε = 0.1729 eV which results in a material melting point of T_L = 1726.8 K with a 0.07 % discrepancy, Pb values of σ = 3.6888 Å and ε = 0.0610 eV which results in a material melting point of T_L = 598.7 K with a discrepancy of 0.32 % and for Cr metal a value of σ = 2.7813 Å and ε = 0.24322 eV resulted in a material melting point value of T_L = 2183.7 K with a discrepancy of 0.17 %.

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