# THERMAL PROPERTIES INVESTIGATION OF FeCr ALLOY USING LAMMPS SIMULATION: A PRELIMINARY STUDY

# *INVESTIGASI SIFAT THERMAL PADUAN FeCr MENGGUNAKAN SIMULASI LAMMPS: STUDI AWAL*

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***Abstrak***

*Saat ini, teknologi reaktor nuklir yang banyak digunakan karena keandalannya yang telah terbukti adalah reaktor nuklir gen-III +. Sekalipun dilihat dari aspek keselamatan dan keandalan reaktor generasi ini sudah terbukti, tetapi karena energi nuklir memainkan peran vital untuk memenuhi kebutuhan energi dunia yang terus berkembang, maka perlu memiliki jenis reaktor nuklir yang disesuaikan dengan kebutuhan tersebut. Generasi reaktor nuklir berikutnya harus memenuhi persyaratan pemenuhan persyaratan keselamatan, fleksibilitas, masa operasi lebih lama (lebih dari 60 tahun), lebih ekonomis. Agar reaktor dapat menghasilkan daya yang lebih tinggi, masa operasi yang lebih lama dan lebih ekonomis, maka diperlukan bahan struktur reaktor yang mampu dioperasikan pada suhu tinggi. Jenis bahan yang diharapkan untuk memenuhi persyaratan ini meliputi berbagai jenis baja feritik / martensit, austenit, baja paduan yang mengandung nikel, dan bahan gelas logam dan bahan keramik. Paduan logam FeCr adalah paduan yang membentuk logam yang disebutkan di atas, sehingga penting untuk melakukan penelitian baik dalam simulasi maupun percobaan. Simulasi Molecular Dynamics dari paduan FeCr menggunakan Large-Atomic / Molecular Massively Parallel Simulator (LAMMPS) skala besar telah dilakukan untuk mengeksplorasi karakteristik termodinamika bahan tersebut di atas seperti perlakuan panas, kelarutan Cr, fungsi distribusi radial atom (RDF). Hasil simulasi diilustrasikan menggunakan kode Visual Molecular Dynamics (VMD).*

Kata kunci : Lammps, baja feritik/ martensit, RDF, VMD

**Abstract**

At present, nuclear reactor technology that is widely used because of its proven reliability is the gen-III + nuclear reactor. Even if it is seen from the aspect of safety and reliability of this generation reactor, it has been proven, but because nuclear energy plays a vital role to meet the growing world energy needs, it is necessary to have a type of nuclear reactor that is tailored to those needs. The next generation of nuclear reactors must meet the requirements of fulfilling safety requirements, be flexible, a longer operating life (more than 60 years), more economical. In order for a reactor to produce higher power, a longer operating life and more economical, reactor structure materials which are capable of being operated at high temperatures are needed. The types of materials that are expected to meet these requirements include various types of ferritic/ martensite steel, austenite, alloy steel containing nickel, and metal glass materials and ceramic materials. FeCr metal alloys are alloys that form the metals mentioned above, so it is important to conduct research both in simulation and experiment. Molecular Dynamics simulation of FeCr alloys using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) has been done to explore their thermodynamic characteristics such as heat treatment, solubility of Cr, atomic radial distribution function (RDF). The results of the simulation are illustrated using Visual Molecular Dynamics (VMD) code.

Key Words : Lammps, ferritic/ martensite steel, RDF, VMD

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## INTRODUCTION

For specific applications, metals are not usually used in their pure form because most pure metals are either too soft, brittle or chemically reactive so that alloying elements are added to modify their properties for special purposes. The presence of a proportion of a second, third, etc. elements associated with a metal to form an alloy, e.g. nickel with iron to form Fe-Ni alloys, can drastically alter some of its properties such as the excellent heat resistant properties and retain their stiffness, strength, toughness and dimensional stability at high temperature. The addition of Cr to form Fe-Cr alloy for high-strength, corrosion-resistant applications. In its pure phase, Cr has BCC crystal structure which is the same with the crystal structure of pure Fe phase. When chromium and iron is used to make an alloy at low temperature, they do not make a complete solid solution caused by the presence of σ–phase and it is usually hard and brittle. On the other hand, when high Cr content FeCr alloy is at a high temperature oxidative atmosphere, oxidation process starts forming $Cr_2O_3$ scale and suppresses the corrosion rate drastically. Corrosion characteristics of 18% and 27% Cr cast iron was investigated [1)]. Based on an ab initio, the stability of small vacancy and vacancy chromium clusters in dilute body-centred cubic (BCC) Fe-Cr alloys were studied [2)] based on the sign change of the enthalpy Cr mixing in BCC Fe. The investigation of magnetic properties of Fe-Cr alloys as a function of Cr content, Cr spatial distribution and its clusters in alloys are analysed [3, 4)] .

Fe-Cr alloys have been regarded as good model alloys for testing various models and theories and used as the basic ingredient in the steel making industry. Fe-Cr based alloys are also regarded as good candidates for the design of various structural components of Generation IV and fusion reactors. Therefore both experimental and theoretical studies of the alloys have been recently intensified. Although many intensive studies on Fe-Cr alloys have been carried out, there are still many things that need to be explored both experimentally and computer simulations such as the diffusion of Fe and Cr under different temperature conditions[5)], to understand and quantify the kinetics and mechanisms of microstructure and property evolution of Fe-Cr alloys under various thermal and ionizing radiation environments etc. [5, 6, 7, 8)]

Some experimental research works on Radial Distribution Function (RDF) using XRD or neutron scattering method have been conducted for different materials [9, 10, 11)]. Pair-distribution function (PDF) analyses or Radial distribution function can be carried out on organic and organometallic compounds from powder electron diffraction data.[12)]

Molecular dynamic (MD) simulation approach can be used to determine RDF of materials at different environment condition. In this paper, Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) MD will be used to simulate RDF of FeCr alloys and discuss some properties that have close relation to RDF in those alloys.

## METHODOLOGY

The FeCr alloys were modelled using empirical potentials calculation methods using the LAMMPS Simulator. All of the calculations were done on Personal Computer PC with Intel (R) Core (TM) i5-4460 CPU @ 3.20 GHz. We used Pre-compiled Windows installers which install LAMMPS executables on a Windows system. VMD has been used for visualizing the diffusion processes and the crystal structures.

MD is a widely used computer simulation method for studying the movement of atoms or molecules in a complex system. The interaction of molecules or atoms for a fixed of time represents the view of the dynamical evolution of the system. To determine the trajectories of the molecules or atoms, classical mechanical Newton's equations are used based on the interatomic potentials between the particles. The simulation process can be briefly described as follows,

The classical equations of Newton's laws are

$$\mathrm{F_i} = \mathrm{m_i a_i} \qquad \text{..... (1)}$$

$$\mathrm{a_i} = \frac{\mathrm{dv_i}}{\mathrm{dt_i}} = \frac{\mathrm{d^2 r_i}}{\mathrm{dt^2}} \qquad \text{..... (2)}$$

$$\mathrm{a_i} = -\frac{1}{\mathrm{m_i}} \frac{\mathrm{dE}}{\mathrm{dr_i}} \qquad \text{..... (3)}$$

The relation between force the potential energy can be illustrated as:

$$\mathrm{F_i} = -\nabla_\mathrm{i} \mathrm{V} \qquad \text{..... (4)}$$

Based on equation (1), (2), (3), and (4) we can obtained V which represents the potential energy of systems.

$$-\frac{dV}{dr_i} = m_i \frac{d^2 r_i}{dt^2} \quad \text{..... (5)}$$

The velocities vi are usually chosen randomly from a Gaussian distribution at a certain temperature. The Gaussian distribution function provides the probability that an atom i has a velocity vx in the x direction at a temperature T.

$$p(v_{ix}) = \left(\frac{m_i}{2\pi k_B T}\right)^{\frac{1}{2}} \exp\left[-\frac{1}{2}\frac{m_i v_{ix}^2}{k_B T}\right] \quad \text{.... (6)}$$

The temperature can be obtained based on the velocities using the relation,

$$T = \frac{1}{(3N)} \sum_{i+1}^{N} \frac{|p_i|}{2m_i} \quad \text{..... (7)}$$

Here N is the number of the atoms in the system [13].

**Verlet Algorithm:** The atomic positions of all atoms is the function of potential energy. However, the potential energy function is complicated in nature and difficult to be solved analytically. Therefore, the motion equation has to be solved numerically. There are many numerical algorithms have been developed mainly Beeman, Verlet, Velocity Verlet, and Leap-frog algorithm [8].

The numerically stable Verlet integrator provides the time reversibility in physical system and prevention of the simplistic form on phase space. Generally, integration algorithms presume the velocities ($v_i$), positions ($r_i$) and accelerations ($a_i$) can be approximated by a Taylor series expansion.

Expanding the position of the $i_{th}$ particle having $r_i$ position at time t + Δt and t - Δt and $b_i$as the third derivative of $r_i$ .

$$r_i(t+\Delta t) = r_i(t) + v(t)\Delta t + \left(\frac{1}{2}\right) a_i(t)\Delta t^2 + \left(\frac{1}{6}\right) b_i(t)\Delta t^3 + O(\Delta t^4)$$

..... (8)

$$r_i(t-\Delta t) = r_i(t) - v(t)\Delta t + \left(\frac{1}{2}\right) a_i(t)\Delta t^2 - \left(\frac{1}{6}\right) b_i(t)\Delta t^3 + O(\Delta t^4)$$

..... (9)

is local error in position of Verlet integrator. Adding the expression (8) and (9)

$$r_i(t+\Delta t) + r_i(t-\Delta t) = 2r_i(t) + a_i(t)\Delta t^2 + O(\Delta t^4)$$

..... (10)

With$a_i = \frac{F_i}{m_i}$, equation (10) becomes:

$$r_i(t+\Delta t) + r_i(t-\Delta t) = 2r_i(t) + \frac{F_i}{m_i}(t)\Delta t^2 + O(\Delta t^4)$$

..... (11)

And we can obtain the Verlet's algorithm for position:

$$r_i(t) = \frac{r_i(t+\Delta t) + r_i(t-\Delta t)}{2} \quad \text{.....(12)}$$

By subtracting equation (8) with equation (9) we obtain:

$$r_i(t+\Delta t) - r_i(t-\Delta t) = 2v(t)\Delta t + \cdots$$

..... (13)

So that the velocity at t can be obtained as :

$$v(t) = \frac{r_i(t+\Delta t) - r_i(t-\Delta t)}{2\Delta t} \quad \text{..... (14)}$$

Using these sets of equations, the positions and the velocities of every particle in the system can be updated over time by iteratively using the old positions and velocities to obtain new positions and velocities over a long period of time until a complete trajectory is obtained [14]

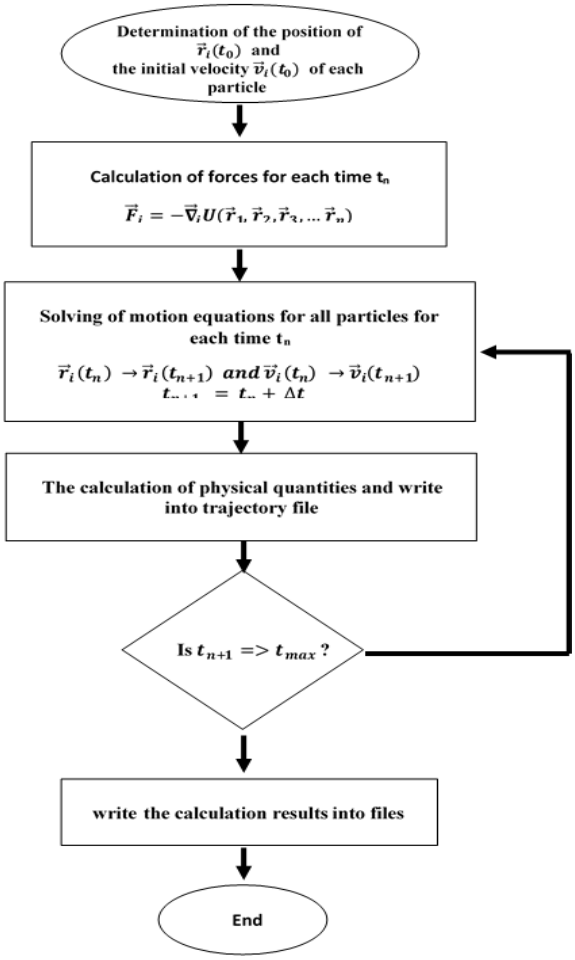


Figure 1.
Flow chart of LAMMPS calculation

LAMMPS is very easy to be used as it is compiled in a specific computational language[15]. Three basic files are needed to run the MD code on LAMMPS platform: input script, a potential file and an exe LAMMPS file. The flow chart of the process of molecular dynamic simulation using LAMMPS is shown in Figure 1.

LAMMPS parameters used in this simulation are shown in Table 1 and the input script has basically four parts;

1). Initialization

Table 1
The parameters used in this simulation.

| No. | Parameter | unit |
|---|---|---|
| 1. | Crystal structure | bcc |
| 2. | Lattice parameter | 2.86 |
| 3. | Potential | FeCr.cdeam Fe Cr |
| 4. | Style | Metal |
| 5. | Ensemble | Npt |
| 6. | Box | 50 x 50 x 50 |
| 7. | Temperature | 300, 450, 2254 K |

The commands for initialization are units, dimension, newton, processors, boundary, atom_style, atom_modify and force−field suc as pair_style, bond_style, angle_style, dihedral_style, improper_style.

2). Atom definition

In LAMMPS, there are 3 ways to define atoms i.e. Read the coordinate of each atom from a data or restart file via the read data, read_restart commands or create atoms on a lattice using these commands: lattice, region, create_box, create_atoms.

3). Setting

Once atoms and molecular topology are defined, a variety of settings can be specified: force field coefficients, simulation parameters, output options, etc. Detail explanation can be read from the LAMMPS manual.

4). Run a simulation

A molecular dynamics simulation is run using the run command such as energy minimization (molecular statics) using the minimize command and a parallel tempering) simulation can be run using the temper command.

In this simulation two works were done namely process of FeCr alloying with different % at Cr and calculation of RDF of FeCr alloy for both crystalline and glassy system. The results of the simulation are illustrated using Visual Molecular Dynamic (VMD) computer program and Excel.

**RESULTS AND DISCUSSION**

a). Visual Molecular Dynamics (VMD) code

Figure 2 Ilustrates the result of simulation using LAMMPS of crystal structure of pure Fe at 300 K. It can be seen that the crystal structure is body center cubic. The lattice spacing is 2.851 A. The result of the simulationis shown by using Visual Molecular Dynamics (VMD) computer program.Visual molecular dynamics (VMD) is a molecular modelling and visualization


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computer program. It is developed as mainly a tool for viewing and analysing the results of molecular dynamics simulations. There are many visualization programs for molecular dynamics simulation results either commercial or open source computer programs. Atom Eye, Para View, OVITO, and VMD are some of open source codes[16].

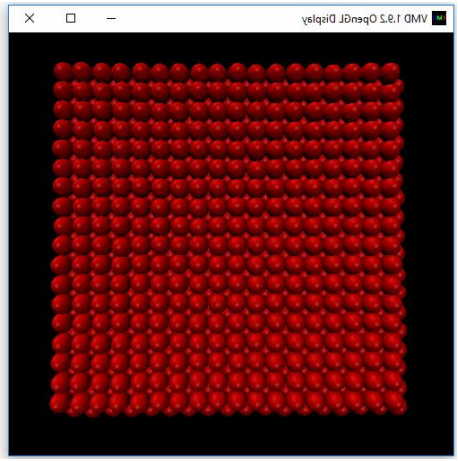
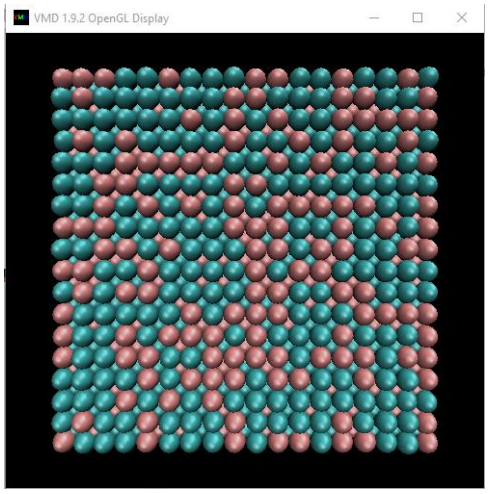
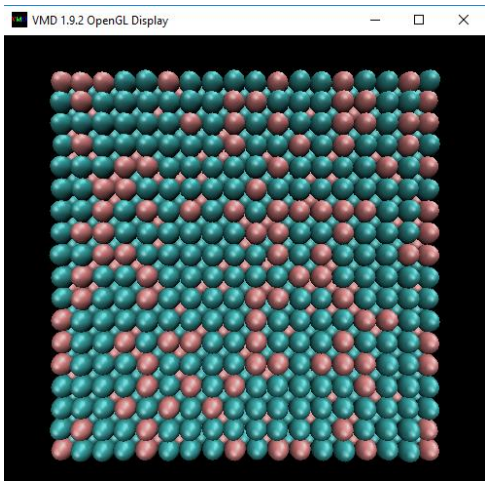


Figure 2.
VMD of pure Fe at 300 K

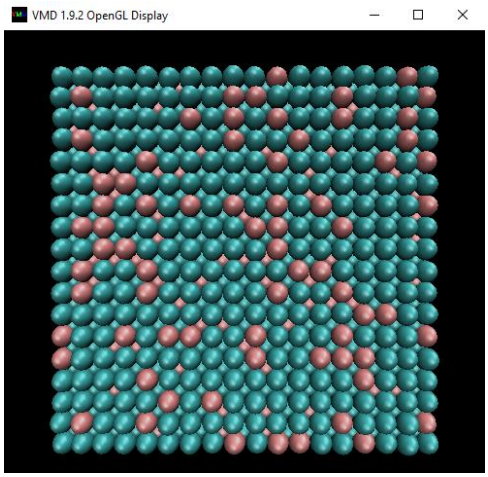
Here, the simulation experiment for making FeCr alloys with different %at Cr was carried out. The results of the simulations are depicted in Figure 3(a), (b)(c) (d) and (e) . The simulations were carried out at the temperatture of 300K. It is seen clearly that from Figure 3(a), (b) and (c) that clusters of Cr precipitate decrease when the %at.Cr decreases. Solubility of Cr atom in FrCr alloy system increases due to the encrease of the temperature. Based on the previous study the solubility limit of Cr in FeCr alloy system was 25% (10%) at Cr at 1000 K (500 K) [17].



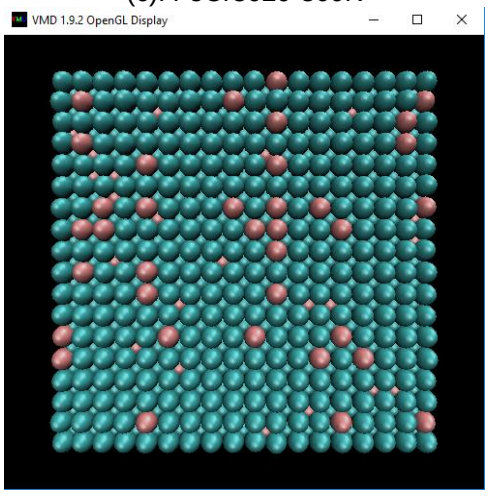

(a).FeCr6040-300K



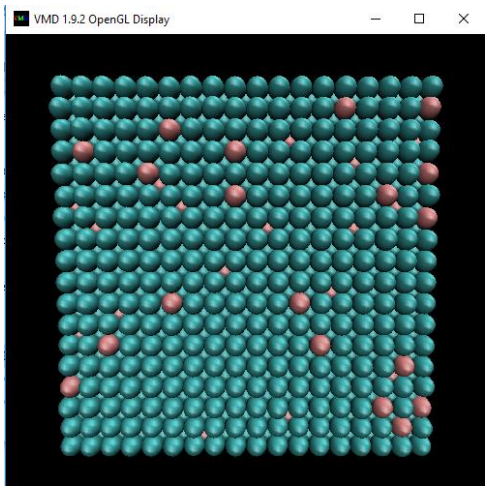

(b).FeCr7030-300K




(c). FeCr8020-300K




(d). FeCr9010-300K




(e). FeCr9505-300K

Figure 3.
FeCr alloy with different % at Cr

b). Volume vs Temperature

Matter usually exists in just three or sometimes four states. They are a solid, a liquid, a gas and rarely a plasma. All matter consists of tiny particles called atoms or molecules. They attract each other to form an equilibrium condition on the environmental conditions characterized by temperature. Those particles are in constant motion. The particles' motion varies due to the pressure, volume, and number of particles. The greater the attraction between the particles, the closer together atomic bonds and their surrounding temperature, volume and pressure.

Here molecular dynamics simulations using the open source software LAMMPS to determine the relationship between volume and temperature of FeCr metal alloy material when the temperature changes was performed.

Figure 4 shows that the higher the temperature of the alloy, the volume will be getting bigger. This is consistent with the nature of the atoms or molecules in a solid phase when energy is added, the atom or molecule vibrates from their initial position so that a new equilibrium is reached and the amount of volume change when the number of particles and the pressure does not change [18]. Lammps can be used to perform simulations to such conditions for a variety of materials in any phase. Simulations can be done by making changes in different temperature, pressure or volume and the thermodynamics and mechanical properties of a material will be obtained. Therefore, this simulation experiments can be performed and obtained the properties of a material with research costs are relatively cheaper compared to laboratory experiments.

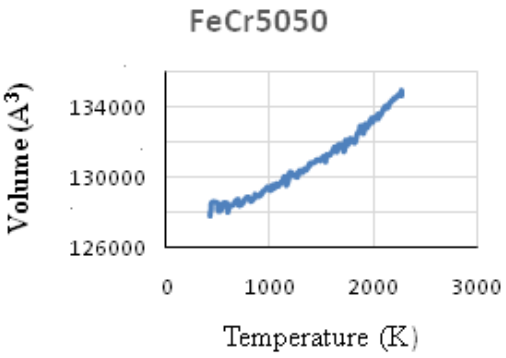
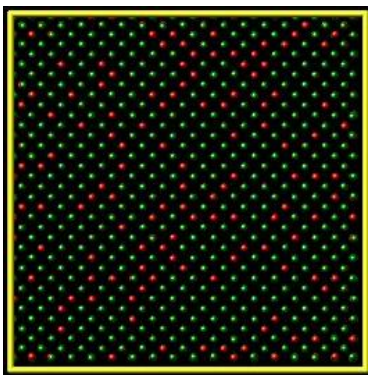
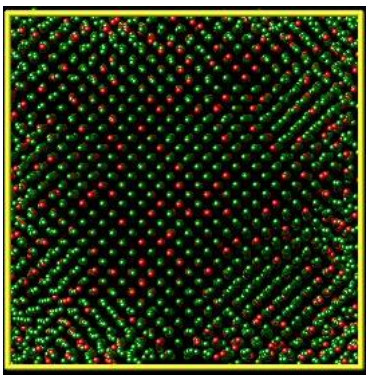



Figure 4
Volume vs. Temperature of FeCr 50%at Cr

c). FeCr8020 alloy at various temperatures



(a). 80%Fe-20%Cr at 300K



(b). 8020-450K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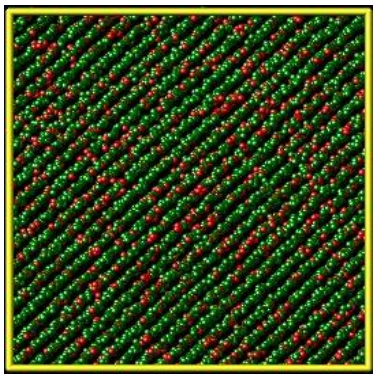


(c). 8020-2254K

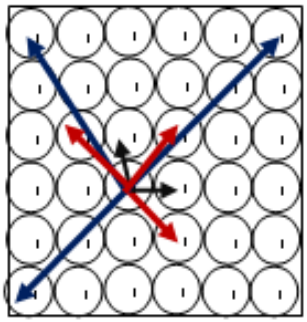
Figure 5.
Heat treatment of FeCr 20% at Cr alloy at various temperatures

By using npt ensemble of LAMMPS, heat treatment process can be done by changing the system temperature i.e. increasing or decreasing temperature. Increasing temperature means adding heat energy to the system. In classical physics, atoms in solid state are arranged in 3-dimensional and connected each other with springs. The system is described by the theories of Newton's laws of motion, Maxwell's equations for the electromagnetic field and the laws of thermodynamics [19]. Based on the theory, objects have a definite position and momentum which can be measured to any degree of accuracy. The system can be simulated and its classical phenomena can be observed. When a crystal system at low temperature, the atoms have a very small kinetic energy so that they vibrate with small amplitude. At low temperature i.e. 300 K, the atoms are illustrated in Figure 5. (a), the vibration of the atoms increases due to the increase of the crystal system temperature. Figure 5. (b), shows that heat energy is added to the crystal system so that its temperature becomes 450 K. It shows here that some atoms start to vibrate with bigger amplitudes while the others are still in the previous condition. It illustrates that the system is at in-equilibrium condition. The simulation is continued by increasing the temperature and it is shown in Figure 5. (c), that all of the atoms vibrate with the bigger amplitudes.

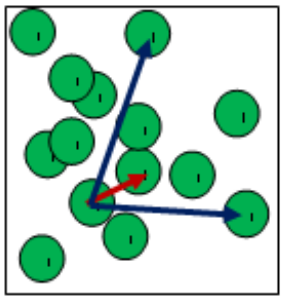
As a result the volume of the crystal system also enlarges in accordance with the increase of the temperature as shown in Figure 4 (with different %at Cr) shown previously.

d). Radial Distribution Function (RDF)

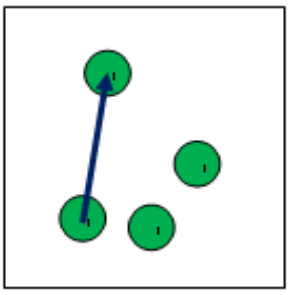
In this study, it was also conducted the simulations for measuring the radial distribution function (RDF) or similarly called distribution pair function (PDF) for FeCr alloy material. RDF can also be obtained experimentally by using either X-ray diffraction (XRD) or neutron scattering. RDF is related to the Fourier transform of the measured scattering intensity S(Q) and in this case it is called as structure function. It is also an important measure because several thermodynamic properties, such as potential energy, pressure and static structure factor can be calculated from it [20]. Moreover, it can also be used to illustrate the phase of matter. Schematically, RDF or g (r) of a matter can be shown such as in Figure 6. When the phase of the matter are in solid (crystal or amorphous), liquid, and gas states.



(a). Solid



(b). Liquid



(c). Gas
Figure 6.
RDF of a matter in (a) Solid, (b) Liquid and (c) Gas

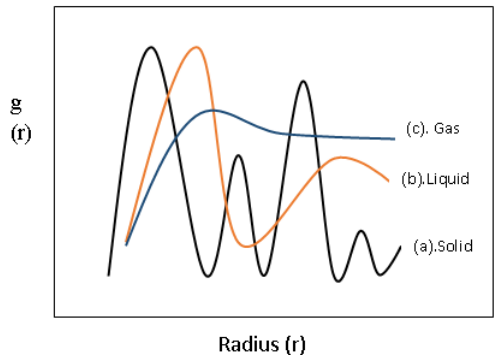



Figure 7. g (r) vs. r curve for (a). Solid (b). Liquid and (c). Gas

In this work, LAMMPS is also used to simulate RDF g(r) of FeCr alloy when the alloy consisted of 50%at.Cr atoms. The simulation was done for two different structures i.e. crystalline and glassy alloy. The results are illustrated in Figure 8. (a) and (b). It can be seen that the results of the simulation are similar to the theory (Figure 7). Figure 7 (a) and 8(a) are similar in having many peaks and it means that they are in crystalline structure where there are many groups of atoms which have same distance from a reference point. On the other hand Figure 7(b) and 8(b) are similar and have two broaden peaks. As illustrated in Figure 6(b) the atoms are not in well order so that only several atoms have same distance to a certain reference point.

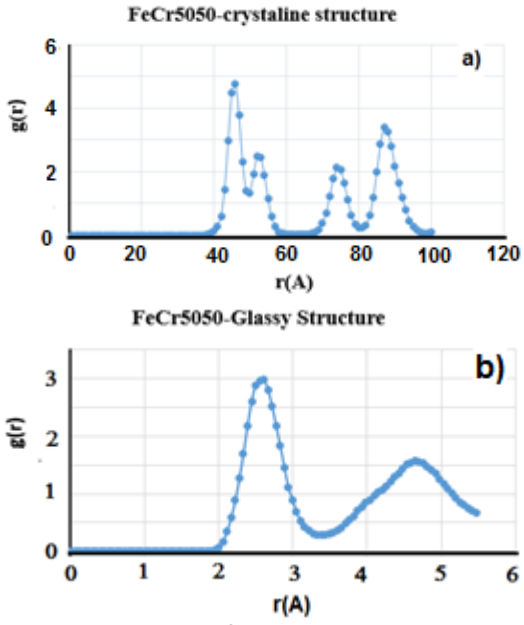



Figure 8.
RDF chart for FeCr 50%atCr (a). Crystalline structure (b). Glassy structure

## CONSCLUSIONS

Thermodynamic characteristics of FeCr alloys have been simulated using Molecular Dynamics simulation of FeCr alloys using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). Some parameters such as solubility of Cr atoms in FeCr alloy, atomic vibration, RDF have been calculated. The simulation results are illustrated using VMD code so that position of atoms can be seen clearly whether they are in crystalline structure or in amorphous structure. From the output of the LAMMPS calculation, the curve of sample volume vs the temperature could be obtained which gives the information of the atomic vibration. From the LAMMPS output, RDF curves could also be obtained which give more detail information about the crystallinity of FeCr alloys. On the other words, when FeCr is heated at high temperature, thermal energy is absorbed and converted into vibration energy so that the FeCr crystal becomes amorphous and it is indicated by broadening of RDF curve and the volume enlarges non-linearly, the greater the temperature the greater the volume change.

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