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Mechanical Properties of Fe, Ni and Fe-Ni Alloy: Strength and Stiffness of Materials Using Lammps Molecular Dynamics Simulation

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Abstract. The mechanical properties of pure metals and alloy Fe-Ni with various compositions have been simulated. The lammps molecular dynamics code was used to compute those physical properties: Ultimate Tensile Strength (UTS) and modulus of elasticity. At temperature 300K the UTS of iron is 8.173 GPa and for nickel is 11.645 GPa. At temperature 300K the elastic modulus of iron is 133.984 GPa and 122.321 GPa for nickel. From the simulation it known that the higher of Ni content, the lower the Ultimate Tensile Strength (UTS) of FeNi alloy and modulus of elasticity. The highest UTS and modulus of elasticity were found in the Fe-5% Ni alloy at the value of 7.960 GPa and 114.978 GPa respectively.

INTRODUCTION

Steel alloy is made from mixture of iron and other atom to make some strong and hard material for specific applications. The strength of steel can be obtained by regulating the percentage of alloying elements such as manganese (Mn), silicon (Si), nickel (Ni), chromium (Cr) and so on. Carbon and other alloying elements can affect the mechanical properties of steel which can increase hardness, scratch resistance and temperature resistance. Heat treatment can affect the microstructure of steel. Metal microstructure is a combination of one or more crystal structures. Metals have a crystalline structure allowing us it to be developed for many potential application [1]. In this work we simulated and compute the mechanical properties of Fe, Ni and FeNi alloy with different compositions. The calculated variables are stress and strain to determine the elastic modulus, UTS (ultimate tensile stress). The simulation was done using LAMMPS molecular dynamics program by lammps.sandia.gov [2].

Material strength is measured by the maximum load that can be received. The tensile stress of steel is the ability of steel to accept the tensile loads given right on the surface area. Testing the tensile strength of a material can be done by giving a tensile load to the test rod slowly until the test material is broken (Daniel, 1985). In this study using a tensile test, which is one of the mechanical stress-strain tests which aims to determine the tensile strength of a material. The effect of temperature variations and various compositions of FeNi mixture is also studied to see the characteristic of material. Material properties can be studied better by using molecular dynamics methods and simulation when reviewed on a molecular scale, where with this scale experiments cannot be observed [3]. Molecular dynamics (MD) method is a computer simulation method based on the analysis of dynamics and interactions of atoms that composing the material but using a macroscopic approach (based on the Newton's 2nd law). Where molecular dynamics methods can function as a bridge between microscopic scale research and macroscopic research in the laboratory. Through calculations by utilizing the mechanics concept, we will obtain the value of physical quantities that we want to know as UTS, elastic modulus etc, based on the trajectory of all particles. Using molecular dynamics simulation, it can produce experimental conditions so that the results of

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calculations on molecular dynamics simulations can be compared with the results of experimental measurement [4,5].

Simulation of mechanical characteristics needs to be done because the design of the new material may need to be characterized by how strong and how flexible the material is so that it can be applied in accordance with the characteristics of the material. For example the bridge design must be made of material that has hard and flexible mechanical properties so that it is not easily broken if given a load or style. This study is to determine the mechanical properties of materials from pure metal material as Fe and Ni and FeNi alloy steel materials. In this work the FeNi alloy will be with content of Ni impurity between 5% and 35%.

The simulation results in this study will be visualized into a strain-stress graph. The UTS are obtained from the highest values of the stress in the linear elastic region of the strain-stress curve.

MATERIALS AND METHOD

Materials

Iron is one type of metal that is often used in various applications. Iron is a chemical element with the symbol Fe, atomic number 26 and is in the first transition metal series of periodic table. Iron has unique properties, namely at high temperatures (> 910 ºC) iron has FCC crystal structure, and at temperatures around 1390 ºC it turns back into BCC crystal structure. Iron has a melting point of 1535 ºC [6].

Nickel is one type of metallic chemical element that is rust resistant. Nickel has a symbol Ni on the periodic table of elements, an atomic number of 28, FCC crystal structure. Nickel has a density of 8.9 g/cm^3 and has a melting point of 1455ºC. This metal has properties that do not change when exposed to air, are resistant to oxidation and have the ability to maintain their original properties under extreme temperatures [7].

Computational Methods

Many computational methods have been used in material researches. The most two popular of these may be the density functional theory (DFT) and molecular dynamics method (MD). Each method has distinct advantages and disadvantages in applications. Generaly the DFT method gives better agreement with experimental data, yet is more computationally demanding than classical MD simulations. Classical MD method may access a broader temperature range and longer time scales in simulation [8]

The DFT have been used to investigate many properties such as Young's modulus and fracture strength [9]. The most significant advantage to DFT methods is a significant increase in computational accuracy. **However, it has** disadvantage of challenge in determining the most appropriate method for a particular application. In DFT there are many functionals available and it is not always clear what is the best choice of functional form for the simulated system under interest? On the other hands the MD method have main advantage that allow obtaining equilibrium macroscopic properties (e.g. temperature, pressure, work, heat, free energy, and entropy), and also the trajectory of the system during the simulation then the dynamical and structural quantities can be obtained [10]

In this work we use the molecular dynamics method to investigate FeNi steels. We learn how the performance of FeNi steel alloys in increasing temperature. This MD method seems to be more appropriate for goal of this work. To run MD simulation, we used the Lammps molecular dynamics program.

Lammps Molecular Dynamics

Lammps (*Large Scale Atomic/Molecular Massively Parallel Simulator*) is one of famous program of molecular dynamics simulation, distributed by *Sandia National Laboratory*, USA. Lammps can simulate material of biopolymers, biomolecules, polymer, solid states as metals and semiconductors [11].

The tensile test is a popular test to know the mechanical properties of material for specific purpose in material applications. This tensile test is often applied for metals, alloys and plastics [12]. In this tensile test, we define the "strain ε" and "the stress σ" [13]. The Fig. 1 is a graph to determine some properties as the UTS and elastic modulus.

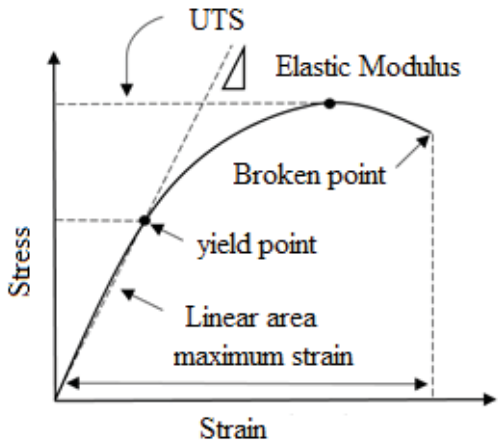

FIGURE 1. Strain-Stress Curve

Conceptly, the stress of material can be calculated by:

$$\sigma = \frac{F}{A_0} \tag{1}$$

where σ is the tensile stress (MPa), F is the tensile force applied to the material (N), and A_0 is the cross-sectional area of the initial specimen (m^2). After a given load F, for example a wire in equilibrium, forces try to pull, shift or suppress it, the shape of the object will change. If the object returns to its original shape after the forces have been removed, the object is said to be elastic. Most elastic objects to forces to their elastic limits [14]

While strain due to the load of static pressure can be determined based on the following equation:

$$\mathcal{E} = \frac{\Delta L}{L} \tag{2}$$

$$\Delta L = L - L_0 \tag{3}$$

where ε is the strain due to attraction, L is the change in specimen length due to compressive load, and L_0 is the length of the original specimen. Through stain and stress analysis it will be known how much the maximum load can be given to prevent the occurrence of fractures [15] It is the strain value has no unit because strain is a coefficient value as in equation (2). Strain due to the attraction, the length will increase, and the diameter of the specimen will be small, a plastic deformation will occur. The relationship of strain and stress can be formulated as follows:

$$E = \frac{\sigma}{\varepsilon} \tag{4}$$

The value of E is the elastic modulus of material, is obtained from the curve gradient in the linear region, where the ratio of stress σ and strain ε is always constant. Curves that state the relationship between strain and stress are often abbreviated as SS curves [15]. More, the effect of temperature on the strain-stress curve was studied by Lu et al.. They explained that an increase in temperature would result in a decrease in yield strength [16]

In Lammps simulation, the stress and strain may be computed by using Lammps utilities “fix…npt” and “fix…deform” as below:

```
fix 1 all npt temp 300 300 1 y 0 0 1 z 0 0 1 drag 1
fix 2 all deform 1 x erate ${strate1} units box remap x
```

For making FeNi steel, its compositions can be varied by using Lammps utility “set group” as:

```
set group all type/fraction 2 0.25 93432
```

For complete example we can see the interesting website [17]. This research was conducted in three stages:

1) The MD simulation with the LAMMPS program. The simulation carried out there are three processes, namely the initiation process, the equilibration process, and the production process. The initiation process is used to determine the system to be used (units, simulation boxes, potential parameters, etc.). The equilibration process is used to obtain a pre-simulation material system for calculating the mechanical properties of materials in a state of minimum energy after being treated for changes in temperature and changes in the percentage of materials. The production process is a simulation that will calculate physical quantities to be analyzed. The simulation is done for pure iron Fe, pure nickel Ni at temperature 300K and FeNi alloy for varied temperatures and compositions.
2) The second stage is to determine and analyze the value of strains and stress materials at a certain temperature or with a percentage of certain ingredients. Determination of strain and stress values was carried out after the process of visualization of the simulation results into a strain-stress graph using the OCTAVE program. [18]
3) The final stage is processing simulation data to determine the characteristics of each test material: calculation of elastic modulus and UTS.

The Lammps script input of FeNi simulation can be done as below script:

```
# ------------------------ INITIATION ------------------------------
units           metal
dimension       3
boundary        p p p
atom_style      atomic
variable latparam equal         2.855           #using lattice constant of Fe
# ----------------------- Geometry of Material -----------------------
lattice                 bcc ${latparam}
region                  whole block 0 25 0 25 0 25
create_box      3 whole
lattice                 bcc ${latparam} orient x 1 0 0 orient y 0 1 0 orient z 0 0 1
create_atoms    1 region whole
set group all type/fraction 2 0.1 93432             #making FeNi structure
mass            1 55.845                            #Fe
mass            2 58.710                            #Ni
# --------------------Potential function--------------------------------
pair_style      eam/alloy
pair_coeff * * FeNi.eam.alloy Fe Ni Fe

#--------------------Equilibration---------------------------------------
compute csym all centro/atom fcc
compute peratom all pe/atom

reset_timestep0
timestep        0.001
velocity        all create 300 12345 mom yes rot no
fix             1 all npt temp 300 300 1 iso 0 0 1 drag 1
minimize        1.0e-4 1.0e-6 100 1000
thermo          1000
thermo_style    custom step lx ly lz press pxx pyy pzz pe temp
run             20000
unfix           1
variable tmp equal "lx"
variable L0 equal ${tmp}
print "Initial Length, L0: ${L0}"

#---------------------Stress-Strain Calculation----------------
reset_timestep0
fix             1 all npt temp 300 300 1 y 0 0 1 z 0 0 1 drag 1
variable        srate equal 1.0e10
```

```
variable        srate1 equal "v_srate / 1.0e12"
fix             2 all deform 1 x erate ${srate1} units box remap x
variable strain equal "(lx - v_L0)/v_L0"
variable p1 equal "v_strain"
variable p2 equal "-pxx/10000"
variable p3 equal "-pyy/10000"
variable p4 equal "-pzz/10000"
fix def1 all print 100 "${p1} ${p2} ${p3} ${p4}" file Fe90Ni.txt screen no
dump            1 all custom 250 *.dump type x y z
thermo          1000
thermo_style    custom step v_strain temp v_p2 v_p3 v_p4 ke pe press
run             20000
#---------------------simulation completely done------------
print "Simulation completed"
```

In above simulation script, we use The EAM FeNi.eam.alloy potential to do run MD Lammps Simulation [19, 20].

RESULTS AND DISCUSSION

Mechanical Properties of Pure Fe and Ni Metals

The simulation done for temperatures of 300K to 600K. Analysis of mechanical properties is focused on mechanical structures that can be observed from stress-strain graphs. The mechanical properties that become the material of analysis are stiffness which can be observed through the calculation of the elastic modulus and the strength of the material that can be observed through the value of Ultimate Tensile Strength (UTS).

Iron simulation

Using input script as described above but for pure Fe metal, the simulation at 300K was done. After some calculation and plotingg using Octave program [18], then the mechanical characteristic of iron at 300K can been shown as Fig. 2 below:

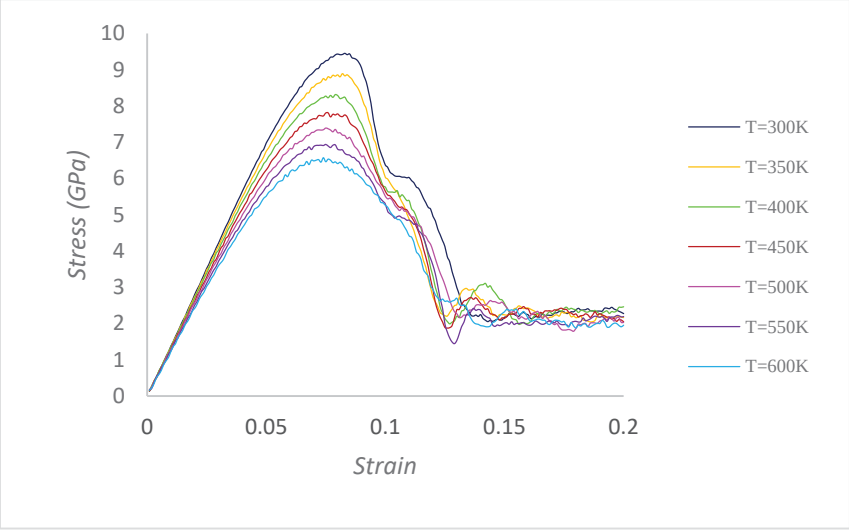

FIGURE 2. Graph of Stress-Strain of pure iron at 300K-600K

From Fig. 2 we can conclude that increasing temperature has an effect on the mechanical properties of the material. Modulus of elasticity (E) can be calculated according to Eq. (4). Table 1 summarize the mechanical properties of iron Fe.

TABLE 1. UTS and Elastic modulus of iron

Temperature (K)	UTS (GPa)	Elasticity Modulus (GPa)
300	8.173	133.984
350	7.589	129.505
400	7.145	124.045
450	6.537	122.876
500	6.209	117.818
550	6.023	112.790
600	5.532	108.898

From Table 1 we see that the elastic modulus of iron decreases for higher temperature. The modulus of elasticity shows how rigid the test material is. The higher the modulus of elasticity, the more rigid the test material will be. This shows that the stiffness of iron will decrease if the simulation temperature is higher. The strength of iron also decreases when the simulation temperature gets higher. This can be seen in Table 1, iron at a temperature of 300K has a UTS value of 8.173 GPa while at a temperature of 350K the iron UTS value drops to 7.589 GPa. This UTS value shows how strong the test material is to withstand the load or external force applied to the test material. The higher the simulation temperature, the more the material will stretch, so that the material will be more elastic due to the smaller atomic bond energy.

Nickel Simulation

Nickel metal analysis is carried out just like the simulation process carried out on iron (Fe). The lattice constant of nickel (Ni) and nickel (Ni) atomic mass are regulated by the programming algorithm of the initiation process. Temperature variations used in this stage simulation as in the simulation for iron (Fe) materials are at temperatures of 300K to 600K. The results obtained after the running of nickel (Ni) can be observed in Fig. 3.

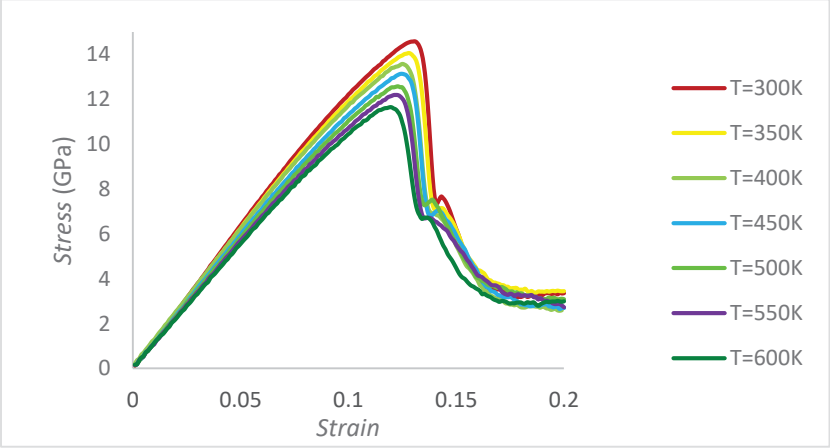

FIGURE 3. Graph of Stress-Strain of pure nickel at 300K-600K

Figure 3 shows the differences in maximum strength of nickel. The higher the simulation temperature, the lower the maximum graph. Seen in Fig. 3, the red graph which is the result of simulation of nickel (Ni) at 300K has a higher Ultimate Tensile Strength (UTS) point compared to the blue graph which is a simulation result at 350K and the red graph also has UTS points are higher when compared to other color graphs that have a higher simulation temperature. This can be seen in the red color chart or the simulation results at 300K have UTS values of 11.645 GPa, while at temperatures above 300K the UTS values are relatively decreased. The results obtained are the same as in the simulation of iron computing, where the strength (strength) of the material is inversely proportional to temperature. The greater the temperature given to the simulation, the lower the strength of the material. The results of the modulus of elasticity and the value of UTS resulting from the simulation of nickel (Ni) can be seen in Table 2.

TABLE 2. UTS and Elastic modulus of nickel

Temperature (K)	UTS (GPa)	Elasticity Modulus (GPa)
300	11.645	122.321
350	11.115	120.553
400	10.710	118.343
450	10.087	115.809
500	9.620	111.596
550	9.339	109.358
600	8.747	107.856

The results of the calculation of the elastic modulus of nickel (Ni) indicate that nickel (Ni) at a temperature of 300K has more rigid properties compared to nickel at temperatures higher than 300K. The modulus of nickel elasticity at 300K is 122.321 GPa, while at temperatures of 350K to 600K the modulus of elasticity of nickel is relatively low.

Fe-Ni Simulation

This study of impurity content was carried out by adjusting the number of particles of Ni in Fe structure. The number of Ni particles making up the simulation material can be created by using "setup group lammps utility" and this can be verified by using "the add modification command" in the OVITO vizualisation tool. So it is necessary to convert the percentage unit of material to provide information on experimental condition [21]. It is informatively if we convert the number of particles (atoms) to weight percentage (wt%) so it can be verified experimentally.

$$x(wt\%) = \frac{m_x \times N_x}{(m_x \times N_x) + (m_y \times N_y)} \quad (5)$$

where x(*wt*%) = wt% of atom x
m_x = mass atom x
N_x = number of atom x in xy alloy
m_y = mass atom y
N_y = number of atom y in xy alloy

The conversion of particle number into weight percentages can be seen in Table 3.

TABLE 3. Compisiton of FeNi alloy

N (Fe)	N (Ni)	wt% (Fe)	wt% (Ni)
20342	10908	63.96%	36.04%
21929	9321	69.12%	30.88%
23428	7822	74.02%	25.98%
25050	6200	79.36%	20.64%
26606	4644	84.50%	15.50%
28157	3093	89.65%	10.35%
29713	1537	94.84%	5.16%

In this study Fe-Ni alloy material will be simulated at a temperature of 300 K, only. The composition of the material can be arranged at the initiation stage. Material composition settings are written with the command "set all type/fraction group" on programming algorithms. The percentage of impurity material used in this study is between 5% and 35% with 5% intervals so that we get 7 variations in the percentage of impurity content. The results obtained after the simulation process can be observed in Fig. 4.

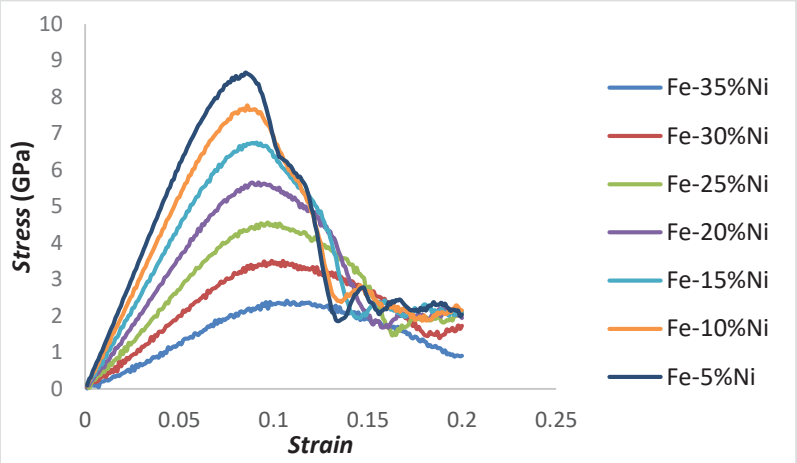

FIGURE 4. Graph of Stress-Strain of Fe-Ni at 300K

From Figure 4 it can be observed that the percentage of impurity content affects the mechanical properties of the material. The smaller the percentage of impurity content, the higher the strength of the test material. UTS values and modulus of elasticity of simulation results can be observed in Table 4.

TABLE 3. The UTS and Elastic Modulus of FeNi alloy

Composition	Temperature (K)	UTS (GPa)	Elasticity Modulus (GPa)
Fe-40%Ni	300	1.280	12.256
Fe-35%Ni	300	2.304	23.837
Fe-30%Ni	300	3.340	37.931
Fe-25%Ni	300	4.285	52.054
Fe-20%Ni	300	5.231	68.300
Fe-15%Ni	300	6.168	84.587
Fe-10%Ni	300	7.045	99.400
Fe-05%Ni	300	7.960	114.978

In Table 4 shows the difference in the value of Ultimate Tensile Strength (UTS) and the modulus of elasticity. The highest UTS value is the percentage of Fe-5% Ni alloy material which is 7.960 GPa. The value of UTS decreases if the percentage of the content of impurity increases. This shows that the higher the impurity content, the lower the strength of the material. Stiffness can be observed through the modulus of elasticity. The greater the modulus of elasticity will result in the material getting stiffer. The alloy of Fe-5% Ni has the highest modulus of elasticity of 114.978 GPa. The modulus of elasticity will be smaller if the percentage of the impurity content is higher. This shows that the higher the percentage of impurity content, the stiffness of the material will be smaller.

The effect of temperature on the stress-stress curve was ever studied by Kumar (2003) who found that increasing temperature would reduce the strength of the material. Decrease in material strength due to increased temperature due to higher temperatures will cause the movement of atoms in material more random. The effect of material composition on the mechanical properties of materials is that the higher the composition of the matrix material (Fe), the higher the value of Ultimate Tensile Strength (UTS) and the modulus of material elasticity. This shows that the higher the percentage of impurity content in Fe-Ni alloy materials, the more strength and stiffness will be.

SUMMARY

In this paper, The mechanical properties of iron (Fe) and nickel (Ni) when the material is treated with temperature variation is the higher the simulation temperature, the lower the Ultimate Tensile Strength (UTS) and modulus of elasticity value. This shows that the strength and stiffness of the material will be lower. The highest UTS values in iron (Fe) and nickel (Ni) metals are at 300K at 8.173 GPa for iron (Fe) and 11.645 GPa for nickel (Ni). Whereas the highest elastic modulus value is at 300K at 133.984 GPa for iron (Fe) and 122.321 GPa for nickel (Ni) metal.

The characteristics of the mechanical properties of Fe-Ni alloys when the material is treated with variations in impurity content is that the higher the impurity content, the lower the value of Ultimate Tensile Strength (UTS) and the modulus of elasticity. This shows that the strength and stiffness of the material will be lower. The highest UTS and modulus of elasticity values were in the Fe-5% Ni alloy at 7.960 GPa for UTS and 114.978 GPa values for the modulus of elasticity.

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