Influence of the Particle Size on the Microstructure and the Curie Temperature (TC) of Nano-Iron Particles Model

Nguyen Trong Dung, Nguyen Chinh Cuong

Abstract*— This paper studies the influence of the particle size (with the chosen sizes 2.122 nm; 2.49 nm; 2.884 nm; 3.128 nm; 3.254 nm; 4.07 nm; 4.68 nm; 4.978 nm; 5.3 nm; 6.602 nm; 7.774 nm; 8.392 nm) on the microstructure and the Curie temperature (Tc) of nano-iron particles model. The nano-iron particles were created by Molecular Dynamics Simulation method with the Pak-Doyama pair interaction potential and aperiodic boundary conditions which is called soft boundary or free boundary. The microstructure characteristics were analyzed through the radial distribution function (RDF), the energy and the coordination number. The Curie temperature (Tc) is the point at which materials switch from the ferromagnetic phase to the paramagnetic phase and it is determined through the Ising model. The study purpose of this paper is to determine the relationship between the particle size and the Curie temperature (Tc) of the model. The obtained results showed that there was specific influence of the particle size on the microstructure and the Curie temperature (Tc) of the nano-iron particles model: when the size of the nano-iron particles was increased from 2.122 nm to 2.49 nm; 2.884 nm; 3.128 nm; 3.254 nm; 4.07 nm; 4.68 nm; 4.978 nm; 5.3 nm; 6.602 nm; 7.774 nm; 8.392 nm, the phase transition temperature of the model increased from 8.9 K to 9.3 K; 9.5 K; 9.6 K; 9.7 K; 10 K; 10.1 K; 10.2 K; 10.3 K; 10.4 K; 10.5 K; 10.6 K respectively. The results have also been compared with the results from the theoretical – experimental model showing the significant influence of the particle size on the Curie temperature of the nano-iron particles model. In addition, the nano-iron particles model at different sizes had the different microstructure characteristics and different Curie temperatures.

Key words: Particle size, microstructure, Curie temperature (Tc), nano-iron particles model, Molecular Dynamics.

I. INTRODUCTION

The nano-ferromagnetic particles have been studied and applied in many devices such as: magnetic sensors [1], data storage devices [2, 3], photo-catalysis [4] and environmental treatment [5]. In addition, they have also been widely applied in biomedicine such as: drug transmission, increasing the contrast for magnetic resonance images, increasing the local hyperthermia and combining with the catalysts to separate the biological molecules [6-9].

The nano-ferromagnetic particles play an important role in biomedical applications for targeted drug transmission by changing the intensity of the external magnetic field to move the magnetic atoms (molecules) with biocompatible coated surface (non-toxic) to the desired location in the body [10, 11], increasing the local hyperthermia [12] as well as marking the cells [13].

When the size of the nano-particles is reduced, they express some distinct properties in comparison with the bulk materials, for example, the magneto-strictive coefficient λ is reduced. The control of the particle size to study the super-paramagnetic of the materials for increasing the magnetism and the interoperability in biomedicine, increasing the heat capacity and reducing the amount of nano-ferromagnetic particles into the body from outside are still the issues to be studied [14]. Therefore, the ferromagnetic-nano particle is regarded as one of the urgent subjects for the scientific research activities [15].

In biomedicine, the use of the nano-ferromagnetic particles with large size will increase the sensitivity of the exposed surface area which makes the phase transition temperature of the materials depend linearly on the particle size [16]. The use of different fabrication methods to create the nano-ferromagnetic particles with different components is beneficial to the researches & applications of the material. The popular experimental methods include the thermal decomposition method [17] and the method of reducing metal salts in organic solvents [18]. Besides the nano-iron particles studies by experimental methods, there have also been the theoretical method such as the Dynamical mean field theory (DMFT) [19].

Today, with the aid of the computer science, the advent of the computers with high-speed and large-capacity memory has led to the significant increase in the model size of the material. To increase the efficiency of the computer technology, the simulation method such as Molecular Dynamics (MD) method has also been applied to determine the microstructure [20-22]; the initial principle method [23-25] and the Monte Carlo method (MC) [26, 27] to determine the magnetism of the nano materials.

The nano-ferromagnetic particle is the material with high magnetic moment (around 220emu/g). When the particle size is smaller than 20nm, it becomes the super-paramagnetic material [28]. In the case of bulk materials, the iron has the face centered cubic (FCC) structure, the Curie temperature ranges from 1183 ÷ 1663K (the phase transition point is around 1096 K) [29]. Therefore, the nano-iron super-paramagnetic particles are useful in the biomedical

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applications at room temperature [30].

In recent years, the experimental results have shown that the changes in the size of the nano particles will lead to the changes in magnetic properties of the materials [31] such as the dependence of the particle size on the Curie temperature (Tc) of the materials [32-36] which has been verified by the theoretical - experimental model. The Curie temperature (Tc) decreases gradually when the size of the material (D) is decreased [32-42]. For nano-ferromagnetic particles, the influence of Tc on D is very significant [43-46]. Based on the experimental results, a number of models has been built and developed to study the mechanism which caused the magnetism of the material [32-42]. The form of the empirical equations has been determined [37].

Besides, there is also another approach by the Ising model to predict the dependence of Tc on D [35]. The development of many models from different perspectives can contribute to the determination of this dependence. However, both theoretical and experimental research results have only been consistent with some specific materials. They have not specifically studied the direct influence of the particle size on the Curie temperature (Tc). Currently, there have been no theoretical results to verify the experimental results but only building and drawing the empirical formulas.

From the above reasons, we have chosen the purpose of this research is to use the Ising model in verifying the dependence of Tc/J on D. The theoretical - experimental model formulas have been used to explain and determine the accuracy of the results. The research has shown that our model has the consistent results with the previous ones [47-57]. The content of the paper includes: Section 1 is the presentation of the latest researches which relate to the content of this paper; Section 2 is the brief presentation of the calculation method; Section 3 is the presentation of the results and discussion; Section 4 is the presentation of our latest conclusions.

II. CALCULATION METHOD

The nano-ferromagnetic particles model with atoms (molecules) was established by Molecular Dynamics model F = m.a (MD). When atoms (molecules) moved, we could verify the elements which influenced the microstructure such as the temperature, the number of particle and the pressure. In the simulation, we chose the Pak-Doyama pair interaction potential (1) with the free boundary conditions which is called the soft boundary or aperiodic boundary [58, 59].

$U(r) = - 0.188917(1.82709 - r)^4 + 1.70192(r - 2.50849)^2 - 0.198294$; $r_c < 3.44A^0$ (1)

in which r(Å) is the distance between atoms; U(r) (eV) is the potential force field; r_c is the disconnect radius.

To determine the microstructure of the nano-ferromagnetic particles, the particles were randomly put in a sphere with the particle size (2) and the density $\rho = 7.0$ g.cm^{-3}.

$$\rho = \frac{N}{V} \rightarrow R = \sqrt[3]{\frac{3N}{4\pi\rho}} \rightarrow D = 2R \quad (2)$$

in which ρ (g.cm^{-3}) is the atomic density; N (particle) is the number of particles; V (cm^3) is the spherical volume; R (Å) is the radius; D (Å) is the diameter or the size of nano particles.

After that, the samples were run statistical recovery with 5.10^5 NPT steps, continuously run with 2.10^6 NVT steps until they reached to the stable temperature of 300 K, then continuously run with 4.10^6 NVE steps until the samples reached to the stable state. After the obtained samples were at the expected stable state, their microstructures were analyzed by determining the influence of the size (2.122 nm; 2.49 nm; 2.884 nm; 3.128 nm; 3.254 nm; 4.07 nm; 4.68 nm; 4.978 nm; 5.3 nm; 6.602 nm; 7.774 nm; 8.392 nm equivalent with the number of particles of 300 particles, 500 particles, 700 particles, 900 particles, 1000 particles, 2000 particles, 3000 particles, 4000 particles, 5000 particles, 10000 particles, 15000 particles, 20000 particles) on the microstructure at temperature 300K. The microstructure characteristics were analyzed through the radial distribution function (RDF), the average energy and the average coordination number. To determine the average coordination number, we chose the disconnect radius $r_c = 3.35$ Å.

After the microstructure was determined, we continued to determine the Curie temperature (Tc) of the nano-iron particles by using the Ising model (3) with the Metropolis algorithm, in which the energy of the model was defined as:

$$E = -\frac{J}{N}\sum_{\langle i,j\rangle}^{N} S_i S_j - H\sum_{i=1}^{N} Si \text{ , H=0} \quad (3)$$

and the other specific quantities of the nano-iron particles were

$$M = \frac{1}{N}\sum_{i=1}^{N} S_i \text{ , } C_v = \frac{\Delta E^2}{k_B T} \quad (4)$$

in which E is the energy of the system; S_k is the spin of k^{th} atom; H is the external magnetic field (H = 0 in the molecular environment); M is the magnetization, Cv is the specific heat capacity.

To study the relationship between the size of the nano-particles and the Curie temperature, we established the relationship between the magnetization and the specific heat of the samples to determine the phase transition temperature of the model. After the nano-iron samples were obtained, all the samples were put into the Ising medium by directing the spin randomly with statistical recovery 10^6 steps, then running 10^6 steps to retrieve the average statistic with disconnect radius $r_c = 3{,}35A^0$ (this value corresponded to the surrounding radius in the crystalline structure).

To verify the accuracy of the simulation results, we used the theoretical - experimental model [60, 61], the formula has the following form:

$$T_c(D) = T_{c0}\exp\left(-\frac{2S_{vid}}{3R}\frac{1}{\frac{D}{6h}-1}\right) \quad (5)$$

with parameters of the nano-iron particles: $S_{vid} = 110.7$ J/g is the melting entropy; h = 0.2482 nm is the atomic diameter; R = 8.314 J/mol.K is Bonzman constant; $T_{C0} = 1044$ K is the Curie temperature of the bulk sample [62, 63]. After the Curie temperature of the nano-ferromagnetic particles model was determined as (Tc/J)

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and the experimental - theoretical model as Tc (D), we determined the dependence of J on D by letting Tc (D) approximate to (Tc /J) and then find J.

III. RESULTS AND DISCUSSIONS

The obtained nano-iron sample has the shape as in Figure 1 and the corresponding sizes in Table 1.

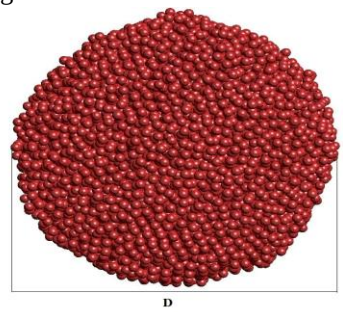


Figure 1. The shape of the nano-iron particles with the size 2.122 nm

Table 1. The sizes of nano-iron samples with different number of particles

Particle number	300	500	700	900	1000	2000
Size D (nm)	2,122	2,49	2,884	3,128	3,254	4,07
Particle number	3000	4000	5000	10000	15000	20000
Size D (nm)	4,68	4,978	5,3	6,602	7,774	8,392

The results in Figure 1 and Table 1 show that the nano-iron sample has the spherical shape and nano size (Table 1). The size of nano particles increases from 2.122 nm to 8.392 nm when the number of particles is increased from 300 to 20000 particles.

Studying the microstructures of the samples, we obtained the results as in Figure 2 and Table 2.

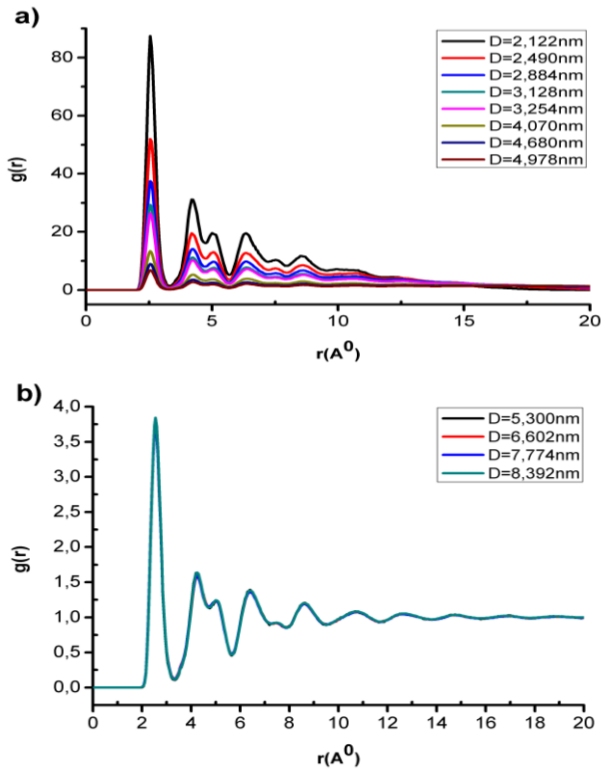


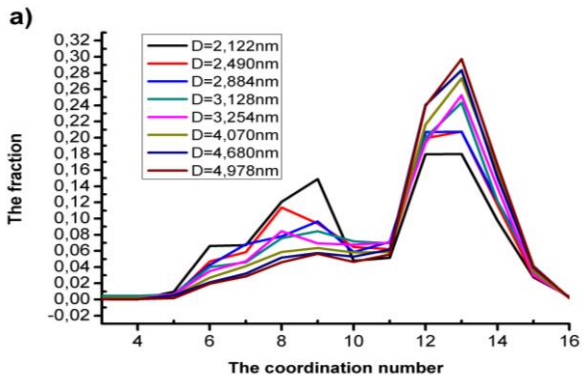
Figure 2. The radial distribution function of the nano-iron samples with the sizes from 2.122 nm to 4.07 nm (Figure 2a) and the sizes from 4.67 nm to 8.392 nm (Figure 2b)

Table 2. The radial distribution function of the nano-iron samples with the sizes from 5.300 nm to 8.393 nm

D (nm)	5,300	6,602	7,774	8,392	TN
r (Å)	2,55	2,55	2,55	2,55	2,56
g(r)	3,834	3,761	3,759	3,839	

The results in Figure 2 and Table 2 show that the first peak position of the radial distribution function predominates in all of the nano-iron samples. When the particle size is increased from 2.122nm to 8.392nm (corresponding to the number of particle from 300 to 20000 particles), we see that the first peak position of the radial distribution function predominates with insignificant changes in values. This result show that the intermolecular distance between atoms (molecules) does not depend on the size or the number of particles. We can conclude that only the near order exists in the couplings between atoms (molecules) of the model. It is noted that the first peak height of the radial distribution function of the samples with particle sizes from 2,122nm to 4.978nm has the great value. It decreases intensively (Figure 2a) when the particle size is increased. For the samples with the sizes from 5.300 nm to 8.392 nm, the first peak height of the radial distribution function has the small value and it is unchanged when the particle size is increased (Figure 2b and Table 2). That indicates the first peak height of the radial distribution function approaches to the unchanged value when the particle size is increased to the value >5 nm, the structure of the obtained sample then have the characteristics of the bulk sample.

Next, we surveyed the coordination number of the samples and the obtained results are shown in Figure 3, the energy of the samples is shown in Table 3.



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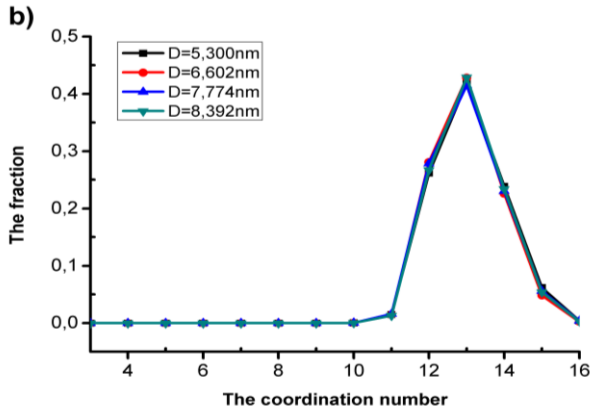

Figure 3. The coordination number of the nano-iron sample at different sizes

Table 3. The energy of the nano-iron sample at the different sizes

Size D (nm)	2,122	2,49	2,884	3,128	3,254	4,07
Energy (eV)	-1,119	-1,158	-1,170	-1,182	-1,191	-1,218
Size D (nm)	4,68	4,978	5,3	6,602	7,774	8,392
Energy (eV)	-1,217	-1,249	-1,254	-1,267	-1,277	-1,285

The results in Figure 3 shows that there are many coordination number 13 and few of coordination number 8. When the particle size is increased from 2.122 nm to 4.978 nm, the density of the coordination number 8 decreases intensively while it increases significantly with the coordination number 13 (Figure 3a). When the particle size is increased from 5.300 nm to 8.392 nm, the density of the coordination number 8 decreases slowly and it increases slowly with the coordination number 13 (Figure 3b). This indicates that the influence of the particle size on the microstructure of the model is due to the heterogeneity. When the size of the sample is greater than 5 nm, the microstructure of the sample tends to be identical with that of the bulk material. We can see from Table 3 that the energy of the sample reduces intensively when the particle size is increased from 2.122 nm to 4.978 nm and it reduces slowly with the particle size from 5.300 nm to 8.392 nm. This indicates the increase in the particle size leads to the increase in the density of atoms (molecules) which makes the density of coordination number 13 increased, the density of coordination number 8 decreased and the energy of the sample reduced gradually. That confirms the increase in the sample size will lead to the increase in the density of the particles which reduces the energy of the sample and lead to the change in the microstructure of the sample.

To study the influence of the particle size on the Curie temperature (Tc/J) of the nano-iron particles model, we studied the nano-iron particles model with the corresponding sizes for the phase transition temperature, the results are shown in Figure 4.

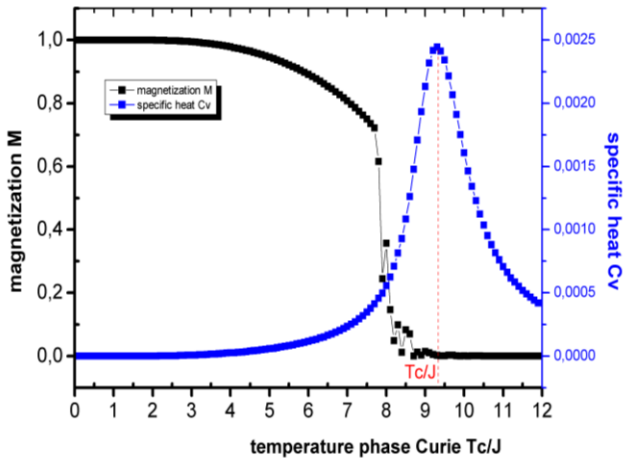

Figure 4. The Curie temperature of the nano-iron sample at the size of 2.49 nm

This result shows that for the sample with the size of 2.49 nm (corresponding to 500 particles), when the Curie temperature (Tc/J) is increased, the magnetization (M) reduces gradually from 1 to zero and the specific heat (Cv) increases gradually. At Tc/J, M approaches to zero and Cv reaches to the maximum value (ie. M = 0, $\frac{dCv}{d(T_C / J)} = 0$).

In addition, when Tc/J increases in the range (7.76; 8.68), M decreases quickly and Cv increases intensively. This proves there are strong changes of M and Cv near the phase transition temperature point.

Studying the influence of the particle size (D) on the phase transition temperature (Tc/J), we obtained the results in Table 4.

Table 4. The Curie temperature (Tc/J) of the nano-iron samples at different sizes (D)

Size D (nm)	2,122	2,49	2,884	3,128	3,254	4,07
Temperature Tc/J (K)	8,9	9,3	9,5	9,6	9,7	10
Size D (nm)	4,68	4,978	5,3	6,602	7,774	8,392
Temperature Tc/J (K)	10,1	10,2	10,3	10,4	10,5	10,6

The above result shows that the phase transition temperature increases rapidly when the size is increased from 2.122 nm to 4.978 nm while it increases slowly when the size is increased from 4.978 nm to 8.392 nm. Thus, when the particle size is from 4.978nm upwards, the phase transition temperature of the model gradually becomes identical to the phase transition temperature of the bulk sample.

We continued to use theoretical - experimental models [60-63] to verify, the results are shown in Figure 5.

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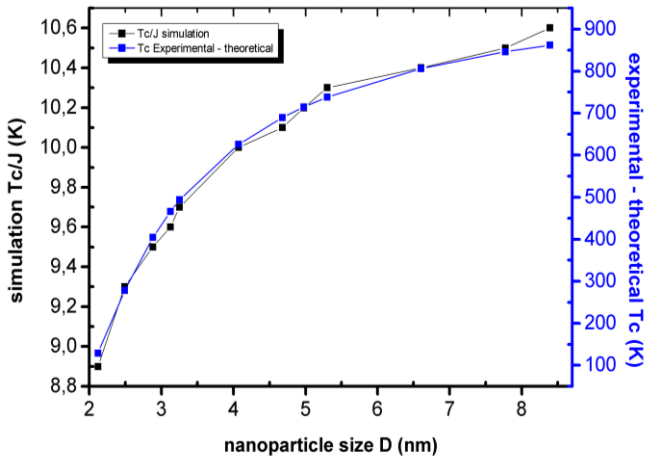

Figure 5. The relationship between the experimental - theoretical Tc and the (Tc/J) of the model when the nano-iron particles samples has different sizes

The results in Figure 5 show that the phase transition temperatures of the theoretical - experimental model and the simulation nano-iron particles model have the identical shapes, there is only small deviation between them. When the particle size is increased, the phase transition temperature of both models increases. When the value of particle size is greater than 5 nm, the phase transition temperatures are identical to that of the bulk sample.

Next, we obtained the values of the exchange integral (exchange energy) which are shown in Figure 6.

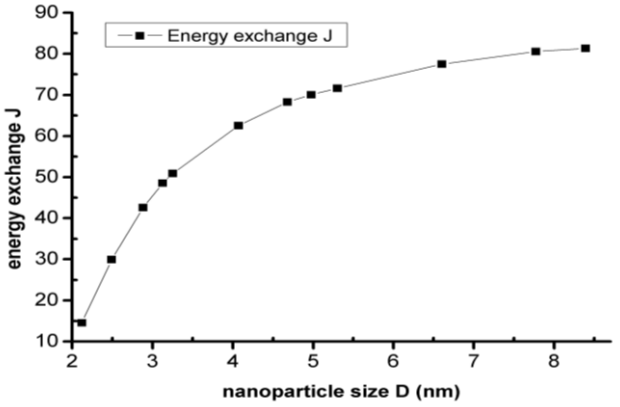

Figure 6. The exchange integral of the nano-iron particles model at different sizes

From Figure 6 we can see that values of the exchange energy of nano-iron particles vary with D. The following polynomial was obtained when the exchange energy of the nano-iron particles was approximately calculated:

J = -0,048D6 + 1,427D5 - 17,148D4 + 107,738D3 - 378,746D2 + 729,915D - 566.952. (6)

This confirms there are significant influences of the particle size on the microstructure and the Curie temperature (Tc/J) of the nano-iron particles model.

IV. CONCLUSION

This paper studies the influence of the particle size on the microstructure and the Curie temperature (Tc/J) of the nano-iron particles model, the following results have been obtained:

-Successfully establishing the nano-iron samples with the sizes of 2.122 nm; 2.49 nm; 2.884 nm; 3.128 nm; 3.254 nm; 4.07 nm; 4.68 nm; 4.978 nm; 5.3 nm; 6.602 nm; 7.774 nm; 8.392 nm by Molecular Dynamics method with the Pak - Doyama pair interaction potential and aperiodic boundary conditions. The results are consistent with previous results [60-63].

-Determine the spherical shape and the nano size of the nano-iron sample.

-Determine the influence of the particle size on the microstructure and the Curie temperature (Tc/J). When the particle size (the number of particles) is increased, the density of atoms (molecules) increases leading to the increase of the interaction between the spins which makes the Curie temperature (Tc/J) increased. The main reason for this result is the size effect, when the number of particles is increased, the size of atoms (molecules) increases which leads to the increase in the coordination number at the surface layer, the core layer and vice versa.

-Determine the main element which influences the Curie temperature (Tc/J) of the nano-iron particles model is the density of the atoms (molecules) in the nano-ferromagnetic particles. The cause of this result is the size effect. When the particle size is increased, the interaction between the spins density increases which makes the magnetism increased and leads to the increase in the phase transition temperature of the nano-iron particles model.

-Determined that there are significant influences of the particle size on the microstructure, the Curie temperature (Tc/J) and the exchange energy of nano-iron particles.

-Determine the coupling between the exchange energy J and the particle size D in the form of a polynomial function.

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