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THE INFLUENCE OF TEMPERATURE ON MICROSTRUCTURE AND THE PHASE TRANSITION TEMPERATURES OF Fe PARTICLE MODELS UNDER SIMULATED CONDITIONS

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Abstract. This paper presents the influence of temperature on microstructure and phase transition when heating 3000 nano-iron and bulk-iron particles at a temperature of 300 K, 500 K, 700 K, 900 K, 1100 K, 1300 K, 1500 K, 1700 K, 1900 K and 2100 K using the molecular dynamics (MD) simulation method. The models were applied in the Sutton-Chen embedded position with the bulk-iron models with the periodic boundary condition and the nano-iron models with aperiodic boundary conditions. The microstructure characteristics of the models were analyzed by using the radial distribution function (PRDF), the average density, the coordination number, the average coordination number and the phase transition temperature of the models was determined based on the temperature dependence of average energy. The results show that temperature influences microstructure and phase transition of the models. For nano-iron models, the phase transition temperature is about 1398 K while it is about 1750 K for bulk-iron models. In addition, the microstructure characteristics of the surface layer and the core layer of the models are different when the models are at different temperatures.
Keywords: Microstructure, phase transition temperature, simulation, Fe models.

1. Introduction

In recent years, the study of the microstructure and phase transition temperature of Fe models using the molecular dynamics (MD) simulation method has lead to a new understanding of nano materials, namely that characteristics and properties of nano material is different from that of bulk material. The reason for this difference is that nano-sized particles are under the influence of quantum effects and surface effects (size

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effect). When the particle size decreases, the total surface area becomes relatively greater and critical effects will occur when the particle size is small enough to compare to the critical size of some properties. Due to the major difference in properties of nano materials, a great many scientists and researchers are involved in efforts to create new materials which have advanced features.

Recently, studies on amorphous Fe models have provided new understandings of material and led to the conclusion that when material is heated to a sufficient temperature, crystallized will occur (at the crystallization temperature, the material is at a state of thermal stability). However, thus far little research has been done on the microstructure of Fe models and the phase transition temperature of the material using the MD method. Previous studies have been limited to influential factors such as temperature, pressure, particle number, duration and diffusion mechanisms. However, studies have not made use of stable technologies, they have not yet identified factors which affects the microstructure of the material [6, 7] and they have not yet determined the phase transition temperature of the material [1-3]. In this report we study in detail the effect of temperature on the microstructure and determine the transition temperature of the models making use of the molecular dynamics simulation method.

2. Content

2.1. Calculation method

According to the simulation results, using Fe models built on the basis of the kinetic equation ($F = m.a$) of the atoms (molecules) [4, 5] when the atoms (molecules) move, the factors that influence the microstructure of the models are temperature, pressure and particle size, and the interaction embedded Sutton-Chen potential [8, 10] was chosen as the most suitable potential for the problem.

$$E_{tot} = \sum_{i=1}^{N} \frac{1}{2} \sum_{j=1, j\neq i}^{N} \Phi\left(r_{ij}\right) + F\left(\rho_i\right) \text{ with } \Phi(r_{ij}) = \varepsilon\left(\frac{a}{r_{ij}}\right)^n$$

$$F(\rho_i) = -\varepsilon C \sum_{i=1}^{N} \sqrt{\rho_i},\ \rho_i = \sum_{j=1, j\neq 1}^{N} \sqrt{\rho r_{ij}},\ \rho(r_{ij}) = \left(\frac{a}{r_{\text{ij}}}\right)^m.$$

Among them: r_{ij} is the distance between the two atoms i and j, F is the interaction force and ρ_i is the i-th electron density. The parameters of the model are presented in Table 1.

Table 1. The parameter values of the Model

ϵ (eV)	a ($\overset{o}{A}$)	N	m	C	R_{cutoff}($\overset{o}{A}$)
0.017306	3.471392	8.137381	4.7877	24.9390	10

In addition to choosing the appropriate interaction potential, it was equally important to choose the appropriate boundary conditions. The free boundary (the boundary region with space surrounded by a vacuum) is applied to nano-iron models and

the periodic boundary (the boundary region in which atoms interact with other atoms on the right, left, top, bottom, front and rear of the space calculations) is applied to bulk-iron models and is oftentimes used for large systems. As computing speed and memory capacity have increased, the research work can be done for the models with bigger sizes [9]. In consideration of factors that affect the microstructure of the model, we choose the molecular dynamics method with the embedded Sutton-Chen potential and boundary conditions at a temperature of 300 K, 500 K, 700 K, 900 K, 1100 K, 1300 K, 1500 K, 1700 K, 1900 K and 2100 K to study the effect of temperature on the microstructure and to determine the transition temperature of the model.

2.2. Results and discussions

Nano-iron models with 3000 particles were heated to a temperature of 300 K, 500 K, 700 K, 900 K, 1100 K, 1300 K, 1500 K, 1700 K and 1900 K with aperiodic boundary conditions, and bulk-iron models with 3000 particles were heated 300 K, 500 K, 700 K, 900K, 1100 K, 1300 K, 1500 K, 1700 K, 1900 K and 2100 K with periodic boundary conditions simulated using the molecular dynamics method with Sutton-Chen embedded position. Each model has the same number of particles, volume and constant energy for thermal stability with 50,000 steps and recovery with 1,000,000 steps until the system reached equilibrium, and the Fe particles obtained had a nano-scale dimension and a spherical shape. Microstructure characteristics of the model, such as location and height of the peak of the radial distribution functions, are shown in Table 2.

Table 2. The radial distribution functions for Iron models (bulk, nano) with 3000 particles at different temperatures

Temp	Bulk radian			Nano radian			Bulk			Nano		
	r_{11}	r_{12}	r_{13}	r_{11}	r_{12}	r_{13}	g_{11}	g_{12}	g_{13}	g_{11}	g_{12}	g_{13}
300K	2.55	4.7	6.9	2.55	4.6	6.75	3.623	1.378	1.237	4.048	1.532	1.311
500K	2.55	4.8	6.9	2.55	4.8	6.85	3.101	1.344	1.160	3.247	1.382	1.212
700K	2.5	4.8	6.9	2.55	4.8	6.85	2.805	1.308	1.123	2.711	1.321	1.133
900K	2.5	4.8	7.05	2.5	4.8	7.0	2.623	1.277	1.090	2.497	1.276	1.128
1100K	2.5	4.75	6.95	2.5	4.9	7.05	2.505	1.253	1.087	2.338	1.257	1.127
1300K	2.45	4.75	7.0	2.5	4.9	7.05	2.384	1.224	1.075	2.254	1.247	1.131
1500K	2.45	4.75	7.0	2.5	4.85	7.1	2.308	1.215	1.069	2.202	1.249	1.145
1700K	2.45	4.8	6.95	2.45	4.95	7.15	2.22	1.191	1.059	2.637	1.469	1.313
1900K	2.4	4.7	6.9	2.45	4.85	7.15	2.137	1.187	1.053	2.442	1.388	1.267
2100K	2.4	4.7	6.9				2.115	1.176	1.045			
Experimental 300K	2.56	4.27	5.01				3.31	1.51	1.18			

It can be seen in Table 2 that the first peak position of the radial distribution function prevails and there is no significant change. This confirms that the bulk-iron and nano-iron

models have no far order in their position, and there always exist a near order in the position of the bulk-iron and nano-iron models. The obtained values for the nano-iron models are very close to those of the bulk-iron models. However, the first peak height of the radial distribution function in the nano-iron models is higher than that of the bulk-iron models. This proves that the density of molecules in the nano-iron models is higher greater than in the bulk-iron models. When the temperature of the models were increased to 300 K, 500 K, 700 K, 900 K, 1100 K, 1300 K, 1500 K, 1700 K, 1900 K and 2100K, respectively, the peak position of the radial distribution function tended to move towards the left side, and this means the average distance of the atoms (molecules) in the models decreased. On the other hand, when the temperature increased, the peak heights of the radial distribution function in both the nano-iron and bulk-iron models gradually decreased. This proves that temperature influences the inconstant structure of Fe particle models. Comparing the results of the nano-iron models in the temperature range of 1300 K to 1900 K with the bulk-iron models in the temperature range of 1700 K to 2100 K, we see that there is difference in the position and in the peak height of the radial distribution function. The peak height of the first radial distribution function is relatively small in comparison with that of the previous temperature range and this means, in terms of microstructure, there is not much difference within this temperature range.

To study this issue in detail, we looked at the average coordination number of the atoms (molecules) in the nano-iron models, which are presented in Table 3.

Table 3. The average coordination number of the nano-iron models at different temperatures

Temp	300K	500K	700K	900K	1100K	1300K	1500K	1700K	1900K
Nano	12.1009	12.0288	11.531	11.0978	10.6392	10.1613	9.8171	9.5357	9.0116

As the temperature increased, the average coordination number of the nano-iron models decreased gradually, which indicates that the average density of the atoms (molecules) in the models decreases.

To confirm this, we study in more detail the coordination number of the nano-iron models at different temperatures, which are presented in Table 4

As the temperature increased, it was seen that the coordination numbers of pairs of atoms (molecules) tended to gradually shift to the left, and the peak intensity also decreased gradually. This proves that the atoms (molecules) have been pulled out of the surface layer of nano-iron models. In addition, the coordination numbers at the surface layer are always smaller than the coordination numbers in the core layer of particles. This is because atoms in the surface layer have smaller coordination numbers than do atoms at the core layer, due to the irreversibility of the process of structure transformation.

To accurately determine the structure transformation points of the above two ranges, we looked at the relationship between enthalpy and temperature, shown in Table 5, Figure 1.

Table 4. The coordination number of the nano-iron models at different temperatures

	300K	500K	700K	900K	1100K	1300K	1500K	1700K	1900K
0							0.0001	0.0002	0.0006
1					0.0002	0.0004	0.0007	0.0015	0.0023
2				0.0003	0.001	0.0027	0.0036	0.0053	0.0072
3			0.0006	0.0019	0.0044	0.008	0.0104	0.0134	0.0171
4	0.0001	0.0005	0.0031	0.008	0.0124	0.0185	0.0214	0.0252	0.0297
5	0.0007	0.0036	0.0119	0.0192	0.0256	0.0312	0.0352	0.038	0.0425
6	0.0079	0.0167	0.0277	0.0352	0.0399	0.0437	0.0455	0.0499	0.0543
7	0.0265	0.0373	0.0451	0.0473	0.0488	0.0516	0.0553	0.0619	0.0721
8	0.0557	0.0582	0.0537	0.0533	0.0551	0.0616	0.0725	0.0855	0.1056
9	0.0761	0.0624	0.054	0.056	0.068	0.0903	0.1101	0.1341	0.1576
10	0.0583	0.049	0.0567	0.08	0.1138	0.1513	0.1729	0.1884	0.1941
11	0.0353	0.0568	0.1008	0.155	0.1894	0.2067	0.207	0.1951	0.1698
12	0.0975	0.1553	0.2098	0.2302	0.2198	0.1878	0.1613	0.1301	0.1003
13	0.2962	0.2778	0.2444	0.1965	0.1495	0.1055	0.0773	0.0548	0.0374
14	0.2735	0.2088	0.1446	0.0916	0.0583	0.0339	0.0224	0.0142	0.0082
15	0.0663	0.065	0.0415	0.0225	0.0124	0.0061	0.0037	0.0022	0.0011
16	0.0057	0.0081	0.0055	0.0028	0.0014	0.0006	0.0004	0.0002	
17	0.0002	0.0004	0.0004	0.0002	0.0001				

Table 5. The relationship between energy and temperature of bulk-iron models and nano-iron models at different temperatures

Temp	300K	500K	700K	900K	1100K	1300K	1500K	1700K	1900K	2100K
	Enthalpy									
Bulk	-2.3282	-2.2716	-2.2202	-2.1697	-2.1218	-2.0810	-2.0335	-1.9895	-1.9430	-1.9076
Nano	-2.2080	-2.1363	-2.0710	-2.0089	-1.9510	-1.8850	-1.8271	-1.7717	-1.7083	

It can be seen that for the nano-iron models, the corresponding phase transition point is at (1398, -1.855) and for the bulk-iron, the corresponding phase transition point is at (1750, -1.968). This shows the strong influence of temperature on the phase transition of the model. For the nano-iron models in which the phase transition temperature is lower than that of the bulk-iron models, when the temperature increased, nano-iron models' structures were increasingly easy to brake in comparison to the bulk-iron models. We see that the values in this temperature range are less variable, and this is consistent with the results observed on the radial distribution functions. Thus, it can be concluded that after the phase transition point, the models converted to a new structure. However, the influence of temperature on this phase transition should be studied in greater detail.

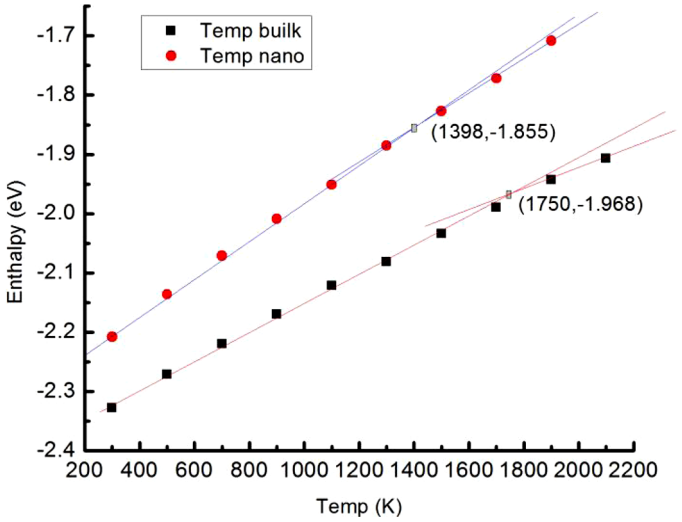

Figure 1. Phase transition temperature of bulk-iron models and nano-iron models with 3000 particles

3. Conclusion

Results obtained from this study looking at the influence of temperature on the microstructure and on the process of verifying the phase transition temperature of Fe particle models using the molecular dynamics method, conducted using 09 nano-iron model samples and 10 bulk-iron model samples at the same temperature of 300 K, 500 K, 700 K, 900 K, 1100 K, 1300 K, 1500 K, 1700 K, 1900 K and 2100 K are as follows:

- Bulk-iron models and nano-iron models with 3000 nano-sized particles were successfully created using the molecular dynamics method with the Sutton-Chen embedded position and the appropriate boundary conditions, and these gave results which were consistent with experimental results.

- A determination was made of the shape of atoms (molecules) in the bulk-iron models and in the spherical nano-iron models which are linked together by electron clouds.

- A determination was made of the influence of temperature on the microstructure of the models. The main structures of the models are Fe atoms (molecules), they concentrate mainly on the core layer of the models and less on the surface layer of the models, and this is a result of the difference in the microstructure of the models.

- The phase transition temperature of the models was determined to be 1398 K for nano-iron models, and 1750 K for bulk-iron models, and these results are consistent with experimental results.

- These results came about largely due to the effect of size. An increase in temperature leads to an increase in the size of the atoms (molecules) and this corresponds to the increased coordination numbers at both the surface layer and the core layer.

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