euspen's 17th International Conference & Exhibition, Hannover, DE, May 2017
www.euspen.eu

Modeling and simulating of high chromium alloy based on Molecular Dynamics

Xiaoguang Guo, Yang Li, Zhuji Jin, Renke Kang
Key laboratory for precision and Non-traditional machining of Ministry of Education, Dalian University of technology, Dalian 116024 China
guoxg@dlut.edu.cn

Abstract
Based on manufacturing process of alloys, a method for constructing the molecular dynamics (MD) model was proposed to study the machinability of a new type of high chromium. The MD model of high chromium alloy was established based on alloy structure with twice atomic random permutation. And then, according to the actual manufacturing process of the high chromium, a quenching process was introduced to simulate the high chromium alloy. The accuracy of the model was verified by calculating the nanohardness and density of the high chromium alloy model after adequate relaxation. Using the new MD model, a series of MD simulations was performed to investigate the nanomechanical property of the high chromium alloy. The results showed that the nanohardness is about 6.951 GPa - 8.095 GPa, and the density is about 7.549 g/cm³, which agreed with the results of actual experimental measurement. The material and the deformation property of the high chromium alloy were stable during the indentation process.
Key words: high chromium alloy molecular dynamics nanoindentation thermal treatment

1. Introduction

With the rapid development of technology, the durability, reliability and precision of mechanical equipment have been put forward higher requirements [1]. High chromium alloy steel is used widely among them because of its excellent properties. Lots of chromium made the high chromium alloy greatly resisted corrosion [2]. Tang X.H [3] studied the volume fraction and microstructure of iron and chromium in high chromium alloy and the wear resistance and corrosion resistance of the high chromium alloy. In the field of mechanical processing, Tabrett C. P[4] studied surfaces of high-chromium white irons, which formed by electro-discharge machining, and analyzed the formation of a re-cast layer, a heat-affected region and extensive surface cracking.

The computer simulation method is more effective than the experimental method to explore the nature of some phenomenon during processing [5]. The MD technology [6], a reliable and powerful computer simulation method on atomic scale, is widely used in the research of nanomachining. Xu S et al.[7] performed large-scale MD simulations of nanoindentation, and studied the mechanical properties as well as wear mechanism of γ-Ti-Al alloy. Henriksson K O E **Error! Reference source not found.** computed the parameters of interatomic interaction in a Fe-Cr-C system, and then explored and fitted the potential for the system.

However, there are not enough researches on the mechanical properties of high chromium alloys in field of MD simulation. On this basis, the model of high chromium alloy was established by MD, and the nanomechanical properties were studied through MD simulation of nanoindentation, and compared with the actual mechanical properties of high chromium alloy.

2. Method

2.1 modeling

The high chromium alloy is a multicomponent alloy. So we selected four elements—Fe, Cr, Ni, C—as the representative elements of the high chromium alloy. Face centered cubic lattice of pure iron was established. According to content of each element in the alloy, the model was built with twice atomic random permutation. A simulation model with 256 000 atoms and size of 14.4 nm × 14.4 nm × 14.4 nm is established. The initial crystal model is shown in Figure 1.

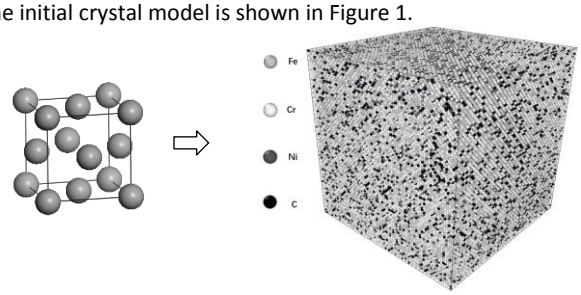

Figure 1. establishing of high chromium alloy steel model

A period of relaxation and the quenching process is needed to make sure that the alloy model is similar to the actual condition as close as possible. During the relaxation, the NPT (isothermal-isobaric ensemble) ensemble is used in simulation system; the initial temperature is 300 K, the pressure is 0 Pa, and three directions of this system are periodic boundary conditions. During the quenching process, the NPT ensemble was used, and temperature of simulation system increased at a rate of 1.8 K/s to 1 200 K, and then dropped to the room temperature at a rate of 4.5 K/s after a period of preservation.

2.2. Potential function

There are a large number of interatomic potential functions to describe the interaction between atoms[9]. EAM (embedded-atom method) potential is the most commonly used to describe the interaction between atoms in alloy, because it can well describe the properties of metals and their alloys[10]. The potential in this work is a hybrid EAM potential. The total energy within EAM is given as:

$$E = \frac{1}{2}\sum_{\substack{i,j=1 \\ j\neq i}}^{N} V_{t_\alpha t_\beta}(r_{ij}) + \sum_{i=1}^{N} F(\rho_i)$$

Where E is the total energy, N is the total number of atoms in the system, $V_{t_i t_j}(r_{ij})$ is the interatomic potential between two atoms, r_{ij} is the distance between the atom i and j, t_α and t_β is the types of element. $F(\rho_i)$ is

embedding energy, atoms embedded in the background of the electron cloud. ρ_i is the sum of the electron density at the i position, which caused by extra-nuclear electrons of all other neighboring atoms except the atom i .

3. Results and discussion

3.1 Verification of Hardness

Nano indentation technology is a good method to study the mechanical properties of materials on the nanoscale. The initial conditions in the nanoindentation simulation are shown in Table 1:

Table1 Nano indentation simulation parameters

Simulation conditions	Simulation parameters
Size of model	14 nm × 14 nm × 4 nm
ensemble	NPT (isothermal-isobaric ensemble)
temperature	300 K
Rate of indenter	10 m/s
Maximum depth of Indentation	2 nm 2.5 nm 3 nm
Time step	1 fs

The pressure of the indenter was recorded during the simulation of the nanoindentation process. It is the resultant force of each atom of workpiece to the indenter. The same indenter of 3 nm (section radius) pressed down to the depth of 2 nm, 2.5 nm and 3 nm at the same rate. The indenters were unloaded after a period of time holding on at each maximum depth of Indentation. According to the relationship between the pressure and the depth of the indenter, the curve was shown in Figure 2.

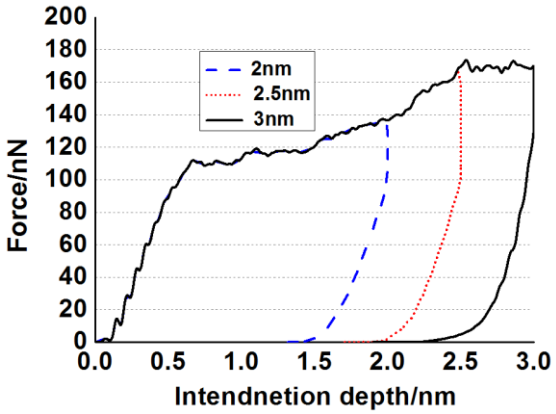

Figure 2. Nanoindentation load displacement curve.

Deformation of the high chromium alloy occurred during the loading progress, elastic deformation was considered in the 0 nm - 0.6 nm of deformation. Curves show that the deformation in the plastic deformation stage and force of indenter increased steadily after 0.6 nm. Both the elastic deformation and plastic deformation stage were all stable, which indicate the high chromium alloy material has a stable deformation law and stable internal properties of the material.

According to the principle of Oliver-Pharr[11] calculation formula of nanohardness:

$$H = \frac{P_{max}}{A}$$

Where H is nanohardness, P_{max} is the maximum pressure during indentation and A is the projected area of the hardness impression.

$$A = 2 \times l \times \sqrt{R^2 - (R-d)^2}$$

Where l is the projected length of the indenter, R is the radius of the indenter, and d is the maximum depth of indentation. The nanohardness of maximum depth 2nm, 2.5nm and 3nm were respectively 6.951 GPa, 7.625 GPa and 8.095 GPa calculated by the formula. The relationship between maximum depth and hardness shown in Fig. 3.

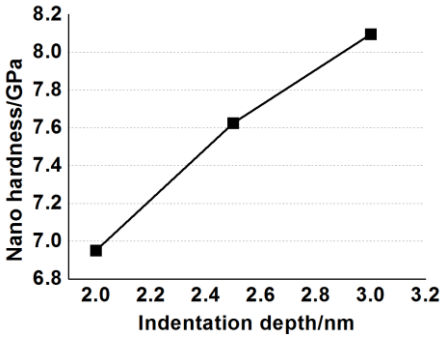

Figure 3. Nano hardness changed curve.

The nanohardness was increasing with the increase of the indentation depth. As the indenter pressed down, the zone of indentation becomes denser and the hardness increases.

3.2 Verification of density

According to the formula $\rho = \frac{m}{V}$, where $m = \sum_{i=1}^{n} m_i$, m_i is the mass of i type atom, the m with calculated is 521.991 g. V is the volume of the alloy model after full relaxation, and there are not lost atoms in the system. The volume of the alloy model is about 691.470 nm³ after full relaxation and heat treatment. The density is 7.549 g/cm³ approximately, and the measured density is about 7.528 g/cm³ actually. Error is about 0.29 %, which shows that the physical properties of the model is very close to that of high chromium alloy.

4. Conclusion

In this work, the model of high chromium alloy was established by molecular dynamics method, and the physical and nanomechanical properties of high chromium alloy were studied. This paper put forward a modeling method of the high chromium alloy, the hardness and density of the model were calculated, the hardness is 6.951 GPa - 8.095 GPa, and the density is 7.549 g/cm³. These properties are very close to the real measured results. Indentation simulation show that the high chromium alloy has a stable material deformation law, which provides a good theoretical basis for the precision and ultraprecision machining of the high chromium alloy.

5. Acknowledgement

The authors would like to acknowledge the financial support from the National Natural Science of China (General Program) (NO.51575083), The National Key Basic Research Program (973 Project) (NO. 2015CB057304), Science Fund for Creative Research Groups (NO. 51621064).

References

[1]. Li W 2000 *J. China Foundry* **5** 597
[2]. Zumelzu E, Goyos I, Cabezas C, Opiz O and Parard A 2002 *J. Mater. Process. Technol.***128** 251-55.
[3]. Tang XH, Chung R, Li DY, Hinckley B and Dolman K 2009 *C. Wear.* **267** 116-21.
[4]. Tabrett CP 1996 *J. Mater. Sci. Lett.* **15** 1792-94.
[5]. Tian J and Liang YC 2001 *C. 7th Equip. Lub. Hyd.* 10.
[6]. Kittel C 2011 *M. Introduction to Solid State Physics* Beijing Chemical Industry Press.
[7]. Xu, S., Wan, Q., Sha, ZD. and Liu, ZS 2015 *J. Comp. Mater. Sci.* **110,** 247–53.
[8]. Henriksson K O E and Nordlund, K 2009 *J. Phys. Rev. B* **79** 14.
[9]. Li HY, Ren XB, Guo XY 2007 *J. Chem. Phys. Lett.***437** 111.
[10]. G. Bonny , N. Castin , and D. Terentyev , 2013 *J. Modell. Simul. Mater. Sci.* **19** 1-14
[11]. Oliver W C, Pharr GM, 2004 *J. Mater. Res.* **19** 3-20