Molecular dynamics study of tensile-compressive behavior of silicon steel single crystal

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Abstract. In this paper, molecular dynamics was used to model and simulate the silicon steel single crystal. The stress-strain curve of silicon steel single crystal in the process of tension and compression and the evolution law of single crystal structure defects in the process of tension and compression were studied. The results show that the tensile strength and compressive strength of the silicon steel model are not similar, the compressive strength is significantly higher than the tensile strength. The compressive strength is about 2 times of the tensile strength. This conclusion is qualitatively verified through macro experiments. The cluster defects and stress show a positive correlation. The number of dislocations in the compression process is more than that in the tension process, but the dislocation size is smaller than that in the tension process. The research in this paper will provide theoretical support for residual stress detection and reduction.

1. Introduction

From smelting to use, metal materials will go through various processes of heat treatment and mechanical processing, such as casting, rolling, welding, cutting, grinding, milling and assembly, etc. After various processing processes, different degrees of stress will be produced inside the metal materials. After these effects and influences are removed, if the stress in the metal components cannot disappear, there are still have some effects and influences remaining in the metal material. This stress in the material is called residual stress. Residual stress is the inherent stress of the material, which belongs to the inherent property of material[2]. Residual stress can distinguished tensile residual stress and compressive residual stress. The existence of tensile residual stress often has adverse effects on material properties, while compressive residual stress can improve material properties. Therefore, the research on the micromechanical properties of materials can provide theoretical support for the detection and reduction of residual stress.

Silicon steel is a very important soft magnetic material. Because of its excellent soft magnetic properties and the advantages of reducing energy consumption, it has broad application prospects in electric power, military, and other fields[3]. Silicon steel is an ideal material to realize the high efficiency and energy saving of electromagnetic equipment. Silicon steel has a low iron loss and high magnetic induction. The content of silicon has an obvious influence on the performance of silicon steel. With the silicon content increases, the iron loss of silicon steel decreases, the magnetic permeability increases, and the magnetostriction decreases. When the silicon content reaches 6.5%, the magnetic properties of silicon steel are the best, that is to say, the magnetic permeability is the largest and the iron loss is the lowest[4]. The mechanical property of silicon steel is also a very important property, which has a very important impact on its service life. Therefore it is very meaningful to study the mechanical properties of silicon steel by molecular dynamics.
Molecular dynamics simulation is based on Newton's second law to describe the movement of a large number of particles in classical dynamics. By solving the motion equation of the whole system, the evolution law of the system with time is obtained based on the theory of statistical mechanics. The length and time scale of molecular dynamics can reach nanometer and femtosecond level, so it is widely used in the study of material properties in nanoscale. The evolution of RTP graphene structure and diffusion behavior of C atoms with cooling rates was calculated. The results show that tailoring the cooling rate could achieve the regular arrangement of distorted structure in as-grown RTP graphene and thus promote the high-quality synthesis of graphene, which was confirmed by the experimental result[5]. Moreover, due to its scale advantage, molecular dynamics simulation can explain the mechanism behind the macroscopic performance behavior of materials from a nano perspective, thus guiding the improvement of experimental preparation technology and the development of material performance control methods. Xie et al. [6] studied three different deformation mechanisms of dislocations under shear loading and revealed that the stability of phase interface is closely related to the interaction of mutually perpendicular misfit dislocation. However, few people currently use molecular dynamics to simultaneously compare and analyze the mechanical properties of single crystal structure in the process of tension and compression.

In this paper, the single crystal model of silicon steel is established based on molecular dynamics. The process of uniaxial tension and compression of the silicon steel single crystal is simulated. The stress-strain curve of the silicon steel single crystal model in the process of uniaxial tension and compression and the evolution law of defects in the model are analyzed. The research in this paper will provide theoretical support for residual stress detection and reduction of technology.

2. Simulation methods
In this paper, the total number of model atoms of silicon steel is 32000. The Fe and Si atoms contained in the model are uniformly distributed randomly. Among them, Si atoms account for 3%, Fe atoms account for 97%. The proportion of other elements in silicon steel single crystal is small, which is ignored in this paper. The size of the model in X and Y directions is 7.06nm, while that in the Z direction is 14.12nm. In order to avoid the influence of boundary effect and simulation scale on the calculation results, the model adopts periodic boundary conditions in X, Y, Z direction to make the model become an infinite ideal nanocrystalline solid[7]. The type of force field is embedded atom MEAM, and the conjugate gradient CG algorithm is used to minimize the energy of the model before tension and compression simulation to optimize the structure of the model and obtain the initialization conditions of the system. The whole process is simulated in LAMMPS molecular dynamics software. The OVITO visualization tool is used to observe the trajectory of the atomic movement. The interaction between Fe and Si is described by 2NN-AlCuFeMgSi -MEAN potential function.

The uniaxial tension and compression deformation law of the model in Figure 1 are simulated. The model uses periodic boundaries for tension and compression in the Z direction. The tension process is simulated by the NVT system. The compression process is simulated by the NPT system (Due to volume expansion occurs during the compression process, the NVT system cannot be used). The model is relaxed at 200ps and the temperature is controlled at 300K to simulate room temperature. In the process of tension and compression, the area of 1nm thickness at the upper and lower ends of the model is fixed. The strain rate of tension and compression is $5 \times 10^{12}$ / s, and the step time is 0.001ps. After the simulation of tension and compression, the stress-strain curves of different models were statistically analyzed. The defects, dislocations, Mises stress (Equivalent stress) of each atom, and displacement in the Z-axis direction were analyzed and calculated by using the OVITO visualization tool.
3. **Analysis on the evolution law of mechanical properties in tension process**

It can be clearly seen from Figure 2 that the energy has stabilized after the 200ps relaxation, indicating that the entire single crystal structure has been stabilized.

The stress-strain curve of the model in the tension process is calculated statistically, as shown in Figure 3. It can be seen from Figure 3 that in the initial elastic stage, the stress increases monotonously with the increase of tensile strain. When the strain reaches 0.18, the single crystal tensile stress reaches the maximum, and the stress is about 18.5 GPa. When the strain exceeds 0.18, the stress of silicon steel single crystal cell changes suddenly, and the complete cell inside the single crystal slips to form dislocation, and then the silicon steel single crystal breaks due to excessive deformation, which indicates that the sliding phenomenon of silicon steel single crystal cell occurs during the tensile to plastic deformation stage. The reason for this phenomenon is the serious lattice distortion effect in the silicon steel single crystal, and also because the silicon steel single crystal contains two different elements, so the lattice distortion is more serious. During the tension process, the single crystal cell is easy to slip, which leads to the large maximum tensile stress and small maximum strain when yielding occurs.

**Figure 1.** Molecular dynamics model of silicon steel single crystal.

**Figure 2.** Energy changes during relaxation.

**Figure 3.** Stress-strain curve of silicon steel single crystal during the tensile process.

**Figure 4.** Displacement variation of silicon steel single crystal during the tension process.
Figure 5. Stress variation of silicon steel single crystal during the tension process.

Figure 6. Defects variation of silicon steel single crystal during the tension process.

Figure 7. Dislocation variation of silicon steel single crystal during the tension process.

During the tension process, the displacement distance in the Z-axis direction, Mises stress, defect, and dislocation of each atom are shown in Figure 4-7. The red part in Figure 4 and Figure 5 respectively represents the atom with larger Z-direction displacement and Mises stress, and the blue part is opposite of the red part. It can be seen from Figure 4 that when the strain reaches 0.1, the
atomic distance between the two ends is very large, and the moving distance is about 1.4nm. However, the single crystal structure is intact at this time, and it is still in the stage of elastic deformation. With further stretching, when the strain reaches 0.2, the upper and lower parts of the model move farther away, and the single crystal has completely broken and failed at the middle and lower parts of the single crystal. Figure 5 shows the Mises stress distribution of each atom in the tensile process of silicon steel single crystal. The redder the color, the greater the atomic stress. When the strain is 0.1, the single crystal is in the elastic deformation stage and the internal stress of the single crystal is relatively small. When the strain reaches 0.2 or later, the single crystal has broken. Although the maximum stress position has been exceeded, the stress concentration phenomenon can still be found in the fractured part of the model, but the stress basically does not change too much, which indicates that when the strain exceeds the maximum stress position, the single crystal color becomes lighter due to the release of fracture stress. There is only one fracture of silicon steel single crystal, which is located in the middle and lower part of the model. The port is regular and flat, which indicates that the silicon steel single crystal has high brittleness and strong hardness.

In order to find out the reason for the change in the number of defects in the model during the tension process, the structure analysis of the model using DXA (location extraction algorithm). The analysis results are shown in Figure 6 and Figure 7. Figure 6 shows a schematic diagram of the changes in defects (cluster) during the tension process. Except for the case where there are no defects in the most primitive ideal state, the defects exist in the entire process of the external influence on the crystal structure. There is a positive correlation between defects and the stress in the single crystal. The stress increases when the defects increase, and the stress decreases when the defects disappear. It can be seen that the defects increase with the increase in strain during the elastic deformation stage. When the structure is destroyed, the defects are reduced, and the defects are mainly distributed near the fracture. It can be clearly seen from Figure 7 that with the change of tension strain, the dislocation first increases and then decreases. The number of dislocations is small, but the size is large. The generation and movement of dislocations will lead to the generation of larger defects in the model, and eventually form dislocation, which leads to a sharp increase in the number of internal defects in the material.

4. Analysis on evolution law of mechanical properties in the compression process
The stress-strain curve of the model in the compression process is calculated statistically, as shown in Figure 8. It can be seen from Figure 8 that in the initial elastic stage, the stress increases monotonically with the increase of compressive strain. When the strain reaches -0.16, the single crystal compressive stress reaches the maximum, and the stress is about -43.9 GPa. When the strain exceeds -0.16, the stress of silicon steel single crystal changes abruptly, and the complete cell inside the single crystal slips to form dislocation, and then the silicon steel single crystal breaks due to excessive deformation, which indicates that the sliding phenomenon of silicon steel single crystal occurs during the compressive to plastic deformation stage. The reason for this phenomenon also is the serious lattice distortion effect in the silicon steel single crystal, and also because the silicon steel single crystal contains two different elements, the lattice distortion is more serious. During the compression process, the single crystal cell is easy to slip. Compared with the tension process, the sliding caused by compression is more severe, which leads to a larger maximum compressive stress and a smaller maximum strain when yielding occurs. As shown in Figure 8, the small wave peaks appearing on the curve when the strain is -0.06 may be caused by the transformation of the single crystal structure[8].
Figure 8. Stress-strain curve of silicon steel single crystal during the compression process.

Figure 9. Displacement variation of silicon steel single crystal during the compression process.

Figure 10. Stress variation of silicon steel single crystal during the compression process.

Figure 11. Defects variation of silicon steel single crystal during the compression process.
Similarly, during the compression process, the displacement distance in the Z-axis direction, Mises stress, defect, and dislocation of each atom are shown in Figure 9-12. It can be seen from Figure 9 that when the strain reaches -0.1, the atomic distance between the two ends is close, and the moving distance is about 1.4nm, at this time, the single crystal structure is in elastic deformation stage. With further compression, the upper and lower parts of the model move closer, and the cross-sectional area continues to expand rapidly. Figure 10 shows the Mises stress distribution of each atom in the compression process of silicon steel single crystal. Similarly, the redder the color, the greater the atomic stress. In the process of compression, the compressive stress in the single crystal increases with the increase of compressive strain. When the strain is -0.1, the single crystal is in the elastic deformation stage, and the internal pressure stress of the single crystal is relatively small. However, when the strain reaches -0.2 or later, the single crystal has rapidly exceeded the yield and reached the plastic deformation stage. At this time, the structure has been damaged. Although the maximum stress position has been passed, the stress of the overall model has decreased with continuous compression, but there is still a phenomenon of stress concentration. The stress of single crystal basically does not change much, which indicates that the single crystal exceeds the maximum stress position, and then the single crystal color becomes lighter due to the stress release due to plastic deformation.

Similarly, in order to find the reason for the change in the number of defects in the model during the compression process, the structure analysis of the model using DXA (location extraction algorithm). The analysis results are shown in Figure 11 and Figure 12. Figure 11 shows a schematic diagram of the change of defects (cluster) in the compression process. It can be seen that the defects in the elastic deformation stage during the compression process increase as the strain increases and the stress also increases. When the structure is destroyed, the defects gradually disappear and the stress decreases and stabilizes. It can be seen from Figure 12 that there is no dislocation line in the model before plastic deformation, but when it exceeds -0.17, the dislocation line starts to appear in the model. This result is consistent with that in the tensile process, and all dislocations appear after plastic deformation. It can also be clearly seen from the figure that with the change of strain, the dislocation first increases and then decreases. The number of dislocations is large, but the size of the dislocations is small. Similarly, the generation and movement of dislocations will lead to the generation of larger defects in the model, and eventually form dislocation, which leads to a sharp increase in the number of defects in the material.

5. Analysis and discussion
In order to compare the difference between the evolution law of silicon steel single crystal in the process of tension and compression, the variation laws of stress-strain and dislocation defects in the process of tension and compression were compared and analyzed. It can be seen from Figure 3 and Figure 8 that the tensile and compressive strength of silicon steel single crystal in the process of tension and compression is not similar. The compressive strength is significantly higher than the tensile strength, which is about 2 times the tensile strength, which is similar to the reference[9, 10]. This conclusion can effectively explain that when using X-ray diffraction detect residual stress(the method is to measure the lattice spacing of materials to characterize the residual stress, and the measured residual stress belongs to the micro residual stress[11]), it is often possible to detect large compressive residual stress, while it is difficult to detect large tensile residual stress. Use the DXA (dislocation extraction algorithm) structural analysis method to extract the dislocation defects in the
tension and compression process of the model. The results as shown in Figure 7 and 12, it can be seen
that the model will have dislocations generated in the process of tension and compression of the model.
In silicon steel single crystal, the dislocation is rarely observed during the tension process, and the
number of dislocation during the compression process is significantly higher than that during the
tension process. In the process of compression, the internal defects are more likely to migrate and
aggregate to form dislocation, while the formation of dislocation can be significantly inhibited during
the tension process. In order to further analyze the changes of defects and dislocation in the process of
continuous internal cascade collision, the number density and total length of dislocation in the model
are calculated. The dislocation in the tension process is quite different from those in the compression
process. The dislocation produced in the tension process is larger, the number is small, and disappears
quickly. During the tension process, there is only one type of dislocation form of \( \frac{1}{2}<111> \). The
maximum dislocation length is 83.2816, and the number of dislocations included is 3. The dislocation
disappears after the strain exceeds 0.2. The dislocation in the compression process is smaller, the
number is large, and has a longer duration. During the compression process, there are three different
types of dislocation forms in the compression process. The first type dislocation is \( \frac{1}{2}<111> \), the
maximum dislocation length is 61.9845, and the number of dislocations included is 8; the second type
dislocation is \(<100>\), the maximum dislocation length is 5.46441, and the number of dislocations
included is 1. The third type of dislocation is \(<110>\), and the maximum dislocation length is 3.99826,
and the number of dislocations included is 1. The dislocation gradually disappears after the strain
exceeds -0.5. The different types of maximum dislocations produced during tension and compression
are shown in Figure 13 and Figure 14.

Within the material, clusters of small defects move along the dense atoms in the lattice. For simple
metals, small interstitial clusters of atoms will migrate in one-dimensional motion mode. For complex
metals, the movement mode of clusters will change, which may change from one-dimensional motion
to three-dimensional motion mode. In this paper, the cage-model is used to explain the motion
behavior of atomic clusters in the model. In the traditional binary alloy, the secondary elements are
randomly distributed in the lattice points of the single crystal cell. Then, the secondary elements will
form many cages with each other to restrict the movement of interstitial clusters within the cage, the
interstitial clusters will move in one-dimensional mode within the cage. While on the surface of the
cage, it will change the motion mode and present a three-dimensional motion. Assuming that the
proportion of secondary elements is \( c \) (0 \(< c < 50\%\)) and the mean free path is \( \lambda \), then the function
relationship between the mean free path and the proportion of secondary elements can be as follows.

\[
\lambda = A c^{-1/3} + B
\]

where \( A \) and \( B \) are constants that could be obtained by fitting to the concept of the mean free path
(MFP) curve.

According to the functional relationship of equation (1), it can know that the mean free path
decreases with the increase of the secondary element. For traditional binary alloys, the proportion of
secondary elements is less than 50\%, but the secondary elements can still inhibit the major elements.
During the tension process, the distance between atoms increases, and the influence of secondary elements on the major elements decreases, so large dislocation can be produced. However, during the compression process, the influence of secondary elements on the major elements increases, so the dislocation loop is smaller.

In the model, the migration behavior of interstitial clusters caused by tension and compression leads to the phenomenon of the different sizes and number of defects and dislocation. When the interstitial atom clusters in the tension process of the model migrate in a one-dimensional motion, they will leave the cascade collision region, which will reduce the probability of the interstitial atoms and vacancies to combine with each other and disappear, so the remaining interstitial atoms will be more. When the interstitial clusters migrate rapidly from the cascade region to the surface of the material, the local swelling and supersaturation will also be caused, resulting in large dislocation. Therefore, the dislocation is larger in the tension process but disappears quickly. This conclusion is consistent with the reference[12-14]. The generation rule of dislocation in the compression process is opposite to that in the tension process. However, for silicon steel single crystals, high lattice distortion not only inhibits the migration of interstitial clusters but also promotes the recombination and extinction of interstitial nuclear vacancies. Therefore, the final remaining defects of the silicon steel single crystal are smaller compared with single element metals. In conclusion, the different evolution rules of dislocations and defects lead to different tensile and compressive strengths of materials. The research results in this paper show that the change of dislocation before and after residual stress reduction can be regarded as an important detection feature for the characterization of the residual stress reduction effect.

6. Experiment verification
In order to verify the accuracy of the molecular dynamics simulation results, a macroscopic comparison experiment was carried out to produce steel samples with the same cross-sectional area. The experimental parts were all cylinders with a diameter of 6mm. The effective length of the tensile sample was 30mm, and the effective length of the compressed sample was 12mm. The dimensions were shown in Figure 15. The sample preparation requirements were all in line with the standard. The strain rate was the same during tension and compression, which was set to 1mm/min.

![Figure 15. Schematic diagram of the tension and compression sample.](image15.png)

![Figure 16. Tensile experiment results.](image16.png)

![Figure 17. Compression experiment results.](image17.png)
The results of the tension experiment and the compression experiment are shown in Figure 16 and 17. It can be seen from Figure 16 and 17, that the non-proportional tensile stress during the tensile process is about 460 MPa, and the non-proportional compressive stress during the compression process is about 850 MPa. The result shows that the compressive strength is significantly greater than the tensile strength. The compressive strength is about 1.85 times the tensile strength. The experiment results are some different from the 2 times shown in the simulation results, this may be caused by the inherent defects of the macroscopic material in the smelting, manufacturing, and subsequent processing processes. This results in differences in the macroscopic and microscopic stress values and multiples, but the macroscopic and microscopic change trends are consistent. In summary, the experiments in this paper can qualitatively prove the correctness of the molecular dynamics simulation results in this paper.

7. Conclusion
In this paper, the 3D model of silicon steel single crystal was established by using molecular dynamics. The stress-strain curve and the evolution law of defects in the process of tension and compression were studied. The results show that the tensile strength and compressive strength of the silicon steel single crystal are not similar. The compressive strength is obviously higher than the tensile strength, and the compressive strength is about 2 times the tensile strength. This conclusion is proved by macroscopic tension and compression experiments. There is a positive correlation between cluster defects and stress changes. The clusters first increase and then decrease with the change of stress. The dislocation of a single crystal model in the process of tension and compression appears in the plastic deformation stage after the highest stress point. The number of dislocations in the compression process is more than that in the tension process, but the dislocation size in the compression process is smaller than that in the tension process. The results of this paper provide theoretical support for residual stress detection and reduction.

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