PCM 2021
MACAU, CHINA

Molecular dynamics study of tension-compression of silicon steel single crystal

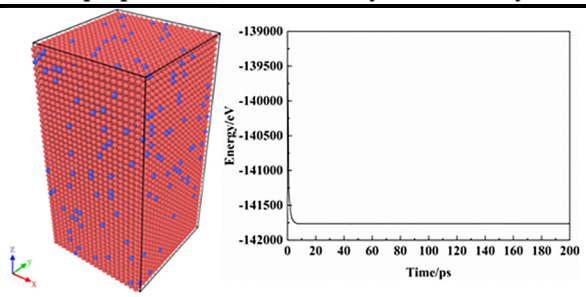
PCM3091

Gang Huang*, Qingdong Zhang, Hao Li

University of Science and Technology Beijing, Beijing , China

Introduction

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. 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. 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.



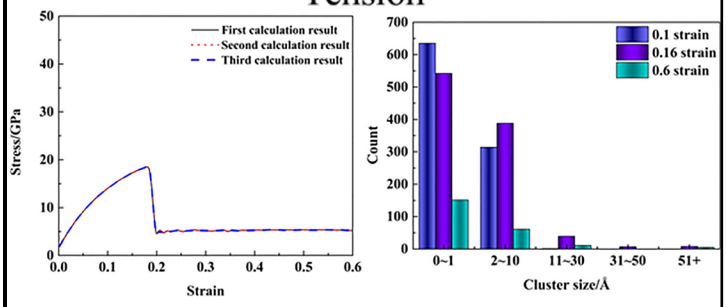
Molecular dynamics model and Energy changes.

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. The model adopts periodic boundary conditions in X, Y, Z direction to make the model become an infinite ideal nanocrystalline solid. The whole process is simulated in LAMMPS molecular dynamics software. The OVITO visualization tool is used to observe the trajectory of the atomic movement.

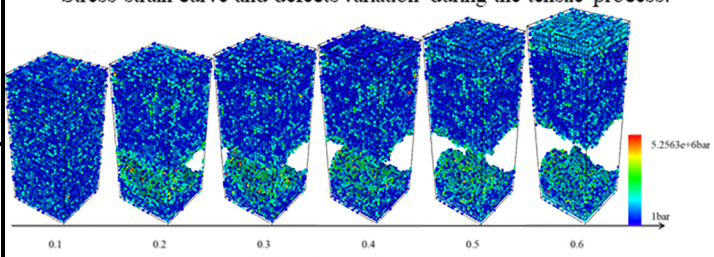
Conclusions

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.

Tension

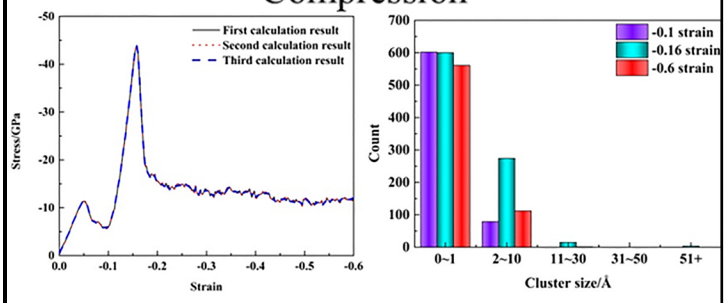


Stress-strain curve and defects variation during the tensile process.

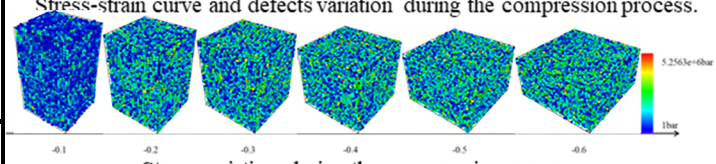


Stress variation during the tension process.

Compression



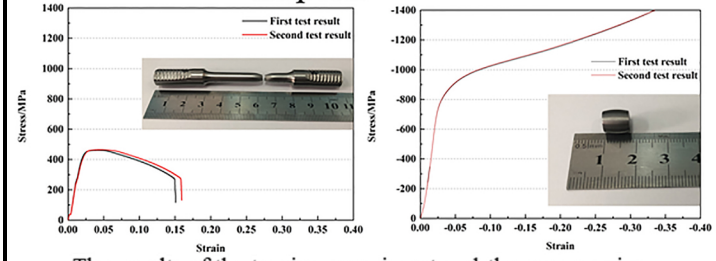
Stress-strain curve and defects variation during the compression process.



Stress variation during the compression process.

The compressive strength is significantly higher than the tensile strength, which is about 2 times the tensile strength.

Experiment



The results of the tension experiment and the compression.

The result shows that the compressive strength is about 1.84 times the tensile strength. In summary, the experiments in this paper can qualitatively prove the correctness of the molecular dynamics simulation results in this paper.

Thanks Beijing Natural Science Foundation (3202019) and QYB