Molecular Dynamics Simulation of Gas Pipeline Steel Based on LAMMPS Parallel Computing Platform

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ABSTRACT

Along with the advent of the fourth industrial revolution, the processing capacity of "big data" is highly demanded in industry community. Compared with the traditional computing and programming model based on serial program, parallel computing is based on heterogeneous architecture and runs in a completely different way from CPU, which has greatly enhanced the processing speed of large-scale data sets. Therefore, parallel computing has been developing dramatically in recent years, and has been favored by all walks of life. In the future, large-scale data processing must belong to parallel computing. Set on LAMMPS (large-scale atomic/molecular massively parallel simulator) as an example, this paper described the technique of establishing parallel computing platform, and applied it on simulated test on fracture process of lamellar structure from gas-pipeline steel.

1. INTRODUCTION

With the advent of the informationalized era, big data, cloud computing and other new concepts come one after another. In the digital environment, data to be processed is also beginning to be quantified in GB or TB. Under the condition that
the domain frequency of CPU is fixed, the computing efficiency of computer decreases obviously when the data sets need to be processed are increasing. Though using classical processing algorithms with excellent performance in various aspects, it is constrained by electronic components and serial algorithms which have reached the physical limit. Hence, the previous methods need longer time to complete the processing of large-scale data. Parallel computing saves a lot of time and space costs by decomposing a computing task into several sub-tasks, then distributing sub-tasks into different processing units. Collaborations among different processing units can solve them quickly. It is predictable that parallel computing will be popular, and will substantially reduce the processing time of data sets.

2. THE PROCESS OF BUILDING A PARALLEL PLATFORM

Although LAMMPS can run on single-processor desktops and laptops, it is designed to run on parallel computers for greater computational efficiency. The LAMMPS molecular dynamics parallel computing platform is based on the Linux operating system (Ubuntu16.04.4) in this time. After the Linux operating system is installed and operated, you need to obtain the corresponding program installation packages. For instance, fftw-2.1.5.tar.gz, mpich-3.2.1.tar.gz, lammps.tar.gz, etc. FFTW is a complete set of fast C programs for implementing discrete Fourier transforms (DFT). It can calculate 1D or multidimensional, real and complex data as well as DFT of any size. The FFTW also includes parallel transformations to distributed shared storage system. The MPICH is installed to build an MPI (Message Passing Interface) programming environment for parallel program development. As for LAMPPS, it is a large-scale atomic and molecular parallel simulator, mainly used for some calculations and simulations related to molecular dynamics. The remaining installation packages involved, such as the voro++ installation package used to calculate the local volume, are installed as needed. The construction process of the LAMMPS parallel compilation part is shown in Figure 1.1.
The compilation of the meam and poems installation packages in LAMMPS needs to be performed after lammps, fftw, and mpich have been installed. The parallel compilation process for the meam and poems installation packages is shown in Figure 1.2 below. After the LAMMPS parallel platform is initially set up, enter the lammps decompression package and enter the crack folder under the example folder to execute the command $ mpirun -n 2 lmp_mpi < in.crack. If it can be calculated, it means that the platform is built successfully, and some calculation process is shown in Figure 1.3.
3. APPLICATION EXAMPLE

3.1 Modeling

A three-dimensional atomic model with a penetrating crack is established in ATOMSK. As shown in the red part of Figure 2.2, the part of cementite model contains 40, 4 and 28 unit cells respectively in three directions. The size of the model is $20.24 \times 2.731 \times 12.628$ nm and it contains 71680 atoms. As shown in the blue part of Figure 2.2 the part of ferrite model whose size is $20.269 \times 2.696 \times 12.638$ nm contains 50, 11 and 18 unit cells respectively in three directions and contains 59400 atoms.

The properties of ferrite-cementite interface are related not only to the crystal structure of ferrite and cementite, but also to the effect of microscopic degrees of
freed at the interface. The first consideration is the terminal type of the crystal at the interface. For ferrite, on account of its highly symmetrical crystal structure, the structure and chemical properties of its termination plane are the same which means there is no need to consider the terminal type of ferrite. Nevertheless, owing to complex oblique crystal structure of cementite, the terminal type needs to be considered. Figure 2. shows eight different cementite termination planes.

3.2 Atomic Simulation Process

3.2.1 SELECTION OF POTENTIAL FUNCTION

The molecular dynamics calculation results are closely related to the selected potential function. In this paper, four typical iron-carbon system potential functions are selected for comparison, including Lennard-Jones/Morse potential function, EAM potential function, Tersoff potential function and MEAM potential function. Considering both accuracy and cost, Tersoff potential function is consequently used in the subsequent simulation process.

3.2.2 RELAXATION TO MINIMIZE ENERGY

The initial crack is prefabricated by eliminating the interaction between the atomic groups throughout the atomic simulation. During the simulation of this experiment, the temperature was kept constant at 300k, and periodic boundary conditions were used in all three directions. In order to select a method to
minimize its energy, it is first tested for experimental conditions. Ma Wen et al. [9], in the molecular dynamics simulation of nano-polycrystalline metal samples, did two-step relaxation to the simulation samples, the static optimization of energy and the NPT dynamics optimization under constant temperature and constant pressure, which effectively reduced the residual stress inside the samples and reached the test state. This can be used as a reference for the energy minimization method in this experiment.

After using the conjugate gradient method to minimize this model’s energy, the NPT constant temperature and constant pressure relaxation of 30 ps with a temperature of 300 K and a pressure of 0 bar is performed. When the relaxation is completed, the model is introduced into OVITO and it is found that in addition to the pre-crack in the middle section, the upper and lower distances between the interfaces no longer exist, and even some ferrite and cementite atoms have merged, as shown in Figure 2.2.

The relaxation calculation gives the average atomic potential energy evolution of the sample and the average atomic kinetic energy evolution of the sample, as shown in Figure 2.3.
drops rapidly at the initial stage of relaxation, it gradually becomes stable after 5 ps, and the average atomic kinetic energy of the sample rapidly rises and stabilizes at an early stage. It can be seen from the figure that from the energy point of view, the energy reaches an equilibrium state after the CG energy minimization and the NPT constant temperature and constant pressure relaxation of 5 ps. Therefore, it is reasonable to use CG energy minimization and NPT constant temperature and constant pressure relaxation of 30 ps.

![Graphs showing the evolution of sample size with relaxation time.](image)

3.2.3 UNIAXIAL TENSION LOADING

Under the NVT ensemble, after the sample is fully relaxed, it is subjected to uniaxial strain tensile loading along the Z direction, and periodic boundary conditions are applied in the X direction and the Y direction to reduce the effect of the size effect. Under the experimental temperature of 300K, the strain rate is $5 \times 10^8$ s$^{-1}$ and the loading step is 1fs. In the simulation process, the atomic information is recorded every 0.2 ps. In order to refine the numerical value of this experiment, when at 0.2 ps the atomic stress and its displacement value are calculated, the average value of the data of 10 time steps near this time is taken as the output value.
3.3 Analysis of Results

Under the condition of 300K, the stress-strain curves of cementite surfaces of the four different terminations under tensile loading are obtained, as shown in Figure 2.4. It can be concluded from the figure that in the uniaxial tensile test, each model undergoes an elastic process in which the stress increases linearly with the load strain. When the critical points are met, the cracks rapidly expand due to the chemical bond rupture between the atoms. The stress gradually drops into the passivation period, and the material failure rapidly occurs, and then the stress gradually decreases to zero. It can also be observed from the figure that the maximum stress values of the C-Fe terminations and the C-C terminations are larger than those of the Fe-Fe and Fe-C terminations, which may be because that the surface is more stable when the carbon atoms are located at the outermost layer of the cementite termination. In the meanwhile, we can see that when the outermost two layers of atoms at the surface termination of the cementite do not contain C atoms, that is, the Fe-Fe termination, not only its maximum principal stress is far smaller than any other termination model’s maximum principal stress, but also it is the one whose stress first decreases to zero and reaches failure state. And the stress is reduced to zero at the slowest speed when the outermost two layers of cementite are all C atoms.

Figure 2.4. Surface models stress and strain relationship diagram.
4. CONCLUSIONS

Compared with the traditional sequential computing method, parallel computing has the advantages of high throughput, low time cost, and resource saving. The steel sheet structure model of α-Fe&Fe3C material was established by LAMMPS and the calculation structure was visualized by OVITO software. Then, the fracture process of the steel sheet structure is simulated, and the microscopic fracture of the steel sheet structure is explored by molecular dynamics method. The molecular dynamics theory was applied to simulate and analyze the material by establishing LAMMPS simulation calculation on the atomic scale of the steel sheet structure. Hence, it can be seen that the LAMMPS molecular dynamics parallel computing platform is extremely applicable and efficient in materials science and computational chemistry.

REFERENCES