3D molecular dynamic simulation of thermodynamic equilibrium problem for heated nickel

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This work is devoted to molecular dynamic modeling of the thermal impact processes on the metal sample consisting of nickel atoms. For the solution of this problem, a continuous mathematical model on the basis of the classical Newton mechanics equations has been used; a numerical method based on the Verlet scheme has been chosen; a parallel algorithm has been offered, and its realization within the MPI and OpenMP technologies has been executed. By means of the developed parallel program, the investigation of thermodynamic equilibrium of nickel atoms' system under the conditions of heating a sample to desired temperature has been executed. In numerical experiments both optimum parameters of calculation procedure and physical parameters of analyzed process have been defined. The obtained numerical results are well corresponding to known theoretical and experimental data.

Keywords: molecular dynamic simulation, nickel, EAM, temperature, thermostat, Newton mechanics equations, parallel algorithm and program, MPI and OpenMP technologies

Трехмерное молекулярно-динамическое моделирование термодинамического равновесия нагретого никеля

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Представленная работа посвящена молекулярно-динамическому моделированию процессов термического воздействия на металлический образец, который состоит из атомов никеля. Для решения этой задачи используется континуальная математическая модель, основанная на уравнениях классической механики Ньютона, выбран численный метод, использующий в основе схему Верле, предложен параллельный алгоритм и осуществлена его реализация в рамках MPIи OpenMP. С помощью разработанной параллельной программы было проведено исследование термодинамического равновесия атомов никеля при условии нагрева образца до желаемой температуры. В численных экспериментах определены оптимальные параметры методики расчета и физические параметры исследуемого процесса. Полученные численные результаты хорошо согласуются с известными теоретическими и экспериментальными данными.

Ключевые слова: молекулярно-динамическое моделирование, никель, ППА, температура, термостат, уравнения Ньютона, параллельные алгоритмы и программы, MPI, OpenMP

1. Introduction

Modern computer equipment makes it possible to simulate very complex systems and processes. Currently, the need for complex systems simulation arises in many branches of knowledge, including in the framework of the nanotechnology implementation in industry. The study of micro- and nano-processes often leads to problems of molecular dynamics of large-scale systems with a large set of uncertain parameters and a variety of conditions that simulate the physical experiment. In this regard, in the last decades new approaches to the modeling of large systems at the molecular level actively develop.

One of the most effective approaches having important fundamental and applied relevance is the method of molecular dynamics (MD) [Kaplan, 1982; Hockney, Eastwood, 1989; Sutmann, 2002; Allen, 2004; Haile, 1992]. The MD method based on a model representation of a polyatomic molecular system in which all the atoms are material points and move according to the laws of classical mechanics. Important areas for the application of molecular dynamics simulation are the design, manufacture and maintenance of the various technical systems, which consist of the metal elements.

In the present work the practical task of computing bases development and carrying out preliminary molecular dynamics simulation of the thermal effects on the sample composed of nickel atoms was set. The novelty of the problem stems from the fact that for nickel new interaction atoms potentials were designed that reproduces more realistically its equilibrium and non-equilibrium states. It gives the chance of carrying out calculations of many technological processes in the microsystems containing nickel coverings at qualitatively new level. In our case, with the help of the research described below preparation for the study of dynamic processes in the micro-nozzles and micro-channels with internal nickel-based alloys will be executed.

To solve the problem of nickel thermodynamic equilibrium calculation the molecular dynamics model was chosen, which is based on the algorithms described in work [Podryga, 2011], the necessary methods of numerical analysis were studied, the estimated parallel program based on specially selected algorithms was created.

2. Problem formulation

In classical molecular dynamics the researched system is represented set of interacting particles. Movements and interactions of the particles are described by Newton's equations. If the particle system is closed, the forces acting on the particles are determined only by the interactions of the particles with each other. These forces are expressed in terms of the gradient of the potential energy with the opposite sign. In case of the external impact on the system presence the forces are the sum of internal and external influences.

In the context of the chosen task it is necessary to research heating of system. For this purpose heat is supplied externally to the system. Thus, the system is not closed. External influence allows to change the system's temperature. The potential energy of system is the sum of the partial interaction energies of particles pairs. Calculation of the pair forces is based on the formulas of the selected interaction potential.

At the initial time the positions and velocities of all particles are set. After that motion equations are solved. For this purpose, on each step forces, new coordinates and velocities of the particles are calculated taking into account boundary conditions and external effects on the system. Solution of the equations system is carried out using finite difference scheme Verlet [Verlet, 1967].

3. Numerical technique

Initial conditions include the distribution of the particle coordinates which has an accurate structure for the solid materials and the distribution of velocities given by the selected starting temperature

of the sample. Nickel has a face-centered cubic lattice (fcc) with the parameter (the edge of the unit cell) which needs to be determined on the basis of the problem conditions (temperature, pressure).

The considered nickel system represents a parallelepiped with the sides Lx, Ly, Lz. $\mathbf{L}(Lx, Ly, Lz) = \mathbf{k} \cdot rcr$ — sizes of the considered area on axes x, y, z respectively, where $\mathbf{k}(k_x, k_y, k_z)$ — quantity of unit cells. Thus, we have a parallelepiped from $k_x \cdot k_y \cdot k_z$ nickel crystals.

The purpose of computer simulation is to obtain estimates of molecular systems consisting of a large number of particles behavior. In case of model calculations are usually restricted to reviewing of the given volume area characteristics at the given density for what enter a molecular and dynamic cell and set periodic conditions on its boundaries. In this work the dynamics of the system examines, in which the axis z of the model is finite, on the other two axes periodicity conditions with periods Lx, Ly of axes x, y respectively are superimposed. In terms of frequency axis z direction is not.

Values of the initial velocity vectors are generated from a Maxwell distribution corresponding to the desired temperature value, for the problem of determining the system relaxation state for the initial it is possible to take value close to the desired value.

The potential energy is represented as a function depending on the coordinates of the particles and describing the interaction between the particles in the system. Selection of a specific type of interaction potential is based on a comparing of the mechanical properties of a computer model of potential and real material. As part of the problem is selected interaction model using the embedded atom model [Daw, Baskes, 1984]. As a function of the pair interaction and density functions were chosen form proposed in [Zhou, Johnson, Wadley, 2004].

Special algorithms — thermostats — are used to maintain the temperature of the system near the set point. Also thermostats are used to achieve the desired temperature and for the relaxation of the system to ensure continuity of the MD calculations at the initial stage. With the relaxation of the system in the case of steady thermodynamic equilibrium temperature of the thermostat and the average temperature of the molecular system must match.

In this paper, Berendsen thermostat and Langevin thermostat were considered to achieve the desired temperature of the system. Berendsen thermostat [Berendsen et al., 1984] is based on the introduction to calculation of sign-variable friction. In modeling the interaction with the heat reservoir is not considered explicitly, but it is defined by the force of friction. Change of kinetic energy is modeled by rescaling the velocities of the system atoms at each step.

Langevin thermostat [Kheerman, 1990] is based on the motion equations of Brownian dynamics. Interaction of system with the heat reservoir is carried out through the introduction of two additional force components comprising a random effect causing heating of the particles and friction forces to compensate for the temperature and prevent overheating of the particles.

An important parameter of the simulation by using the heating thermostat is the interaction time with the heat bath. As a result, consideration of different values of this parameter is determined by the optimal time interaction with the reservoir in the conditions of the problem, due to which the system will reach the equilibrium state in a shorter period of time compared with other values of this parameter.

4. Parallel realization

To implement the developed numerical approach the concept of parallel programming, developed in [Polyakov et al., 2012] was used. It is based on the principles of geometric and functional parallelism. In our case the estimated area breaks into local domains of identical power. Power of the domain is measured in number of elementary boxes, in each of which molecules surely interact with each other. Partition on domains is made within topology a three-dimensional grid. Each estimated domain gets on the calculator as whom the node of a cluster or a supercomputer is used. Distribution of domains on calculators is realized by means of MPI library.

Within a node (calculated domain) is a certain amount of elementary boxes grouped into three-dimensional sublattice. Such a structure is used for further calculations on the distribution of the trade central processing units (CPUs).

The main algorithm of calculation looks as follows.

Step 1 — Read the original data MPI-application and initialize data structures for each calculator.

2nd stage — basic calculations in the cycle time.

3rd stage — the implementation of the resulting calculations and deinitialization.

In the first phase the determination of the molecules number in computational domain, the generation of their location (within the face-centered lattice of nickel), as well as the generation of uniform at the angles and the Maxwell modulus distribution of pulses, the calculation starting forces are carried out.

As part of the main loop the following steps are executed on time. First, the new values of the coordinates are calculated. Next their correction by means of periodic boundary conditions is made. After this particles exchange between the concrete boxes is made, which is carried out within the calculated domain and between domains calculated using the functions MPI.

Further the calculation of the forces on the basis of which the correction is made of particle velocities and calculated all the necessary integral characteristics are calculated. When you reach the control time points the necessary data are stored in files.

Details of the computer implementation are explained more detail in [Podryga, Polyakov, 2014].

Basic test calculations were performed on the Keldysh Institute of Applied Mathematics RAS budget cluster with processors Intel Xeon X5650 @ 2.67GHz and network speed to 2 Gbit/s. The results of acceleration and parallelization efficiency calculations are presented in Table 1. In the calculation of these characteristics the total number involved in the calculation of parallel threads (NT) was used, although the parallelization was performed using hybrid technology that combines MPI and OpenMP. As might be expected, streaming parallelism was not so effective than parallelization across nodes. However, collectively it was succeeded to reduce the time of calculations dozens of times in a relatively small maximum configuration.

Table 1. Data on efficiency of calculations when using technology MPI+OpenMP

Size crystal	24x24x24 (55296 particles)		48x48x48 (442368 particles)		96x96x96 (3538944 particles)	
NT	ACC	EFF	ACC	EFF	ACC	EFF
Budget Cluster						
1	1.000	100.000	1.000	100.000	1.000	100.000
2	1.811	90.529	1.806	90.300	1.844	92.207
4	2.406	60.149	2.496	62.394	2.440	61.009
8	3.074	38.427	2.611	32.637	2.660	33.247
12	**2.943**	**24.528**	**2.917**	**24.306**	**2.967**	**24.727**
16	3.383	21.144	3.141	19.632	3.098	19.361
24	3.495	14.564	3.436	14.315	3.709	15.455
48	7.278	15.162	7.253	15.111	6.936	14.451
96	**13.679**	**14.249**	**12.864**	**13.400**	**13.572**	**14.137**
192	**24.220**	**12.615**	**25.391**	**13.225**	**27.116**	**14.123**
384	**28.812**	**7.503**	**48.385**	**12.600**	**50.572**	**13.170**
Supercomputer K100						
1	1.000	100.000	1.000	100.000	1.000	100.000
12	**5.003**	**41.691**	**5.056**	**42.135**	**5.066**	**42.220**
96	**33.726**	**35.131**	**35.933**	**37.431**	**34.733**	**36.180**
192	**55.386**	**28.847**	**63.010**	**32.818**	**62.627**	**32.618**
384	**77.276**	**20.124**	**97.550**	**25.404**	**107.265**	**27.933**

5. Simulation results

In this section we present some results of the calculations. Determination of equilibrium macro-parameters of nickel system (average temperature, pressure and pulse) and also determination of optimum parameters of numerical algorithm and thermostat were the purpose of calculations. Most of this research has been performed in the framework of [Podryga, Polyakov, 2014]. As a result in numerical experiments optimum parameters of a calculation procedure (an integration step, time of interaction of system with the thermal tank) and also physical parameters of the modeled process were determined (in particular, internal pressure of a sample). The obtained numerical results were compared with known theoretical and experimental data and confirmed a good agreement with the last.

In this paper along with the efficiency of the parallel implementation we were interested in the distribution of pressure and temperature on the sample height depending on the thickness of the controlled temperature layer. For this purpose we selected the sample which is in vacuum with sizes 24x24x24n, where n — number of vertical layers. For example, we took $n = 5$ and considered the situations when thermostat wasn't use and also when the thermostat (in this case Berendsen thermostat was selected) located in the center of a sample and occupied 1, 3 и 5 layers. Length of a crystal edge was equal $a = 0.35311$ nm. The initial temperature of a sample and temperature of the thermostat matched and were equal 273 K. To obtain a stable crystal it is necessary before simulation to work on the determination of the edge length of the unit cell corresponding to the researched temperature and the used interaction potential model. As a result of such work the value of an edge $a = 0.35311$ nm was obtained.

Data of calculations are shown in Fig. 1, 2. Digits 1–4 denote the curves corresponding to the absence of a thermostat (curve 1), and the cases when number of thermostated layers is equal 1, 3 and 5 (curves 2, 3, 4). The figures show that the pressure in the sample is close to zero (i.e., the crystal is stable) irrespective of the thickness of thermostated zone of sample. The temperature in the sample has a parabolic profile corresponding to the thickness of the controlled temperature zone. These data are in agreement with the theoretical concepts of thermal distribution in a bulk sample. In case of simulation of near-surface interactions of a metal sample with an external environment temperature control should be applied in its inside layers not to distort an interaction pattern.
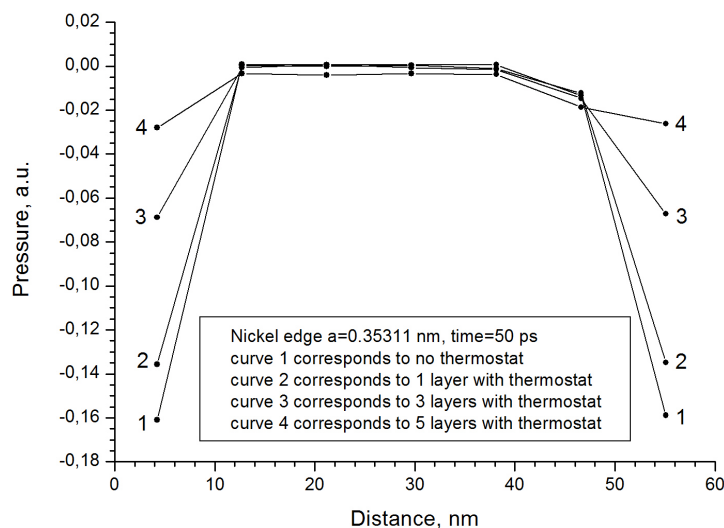

Fig. 1. Pressure distribution over the height of the sample

6. Conclusion

To solve the problem for the establishment of thermodynamic equilibrium in the nickel plate molecular dynamics model was selected, the necessary methods of its numerical analysis were studied,
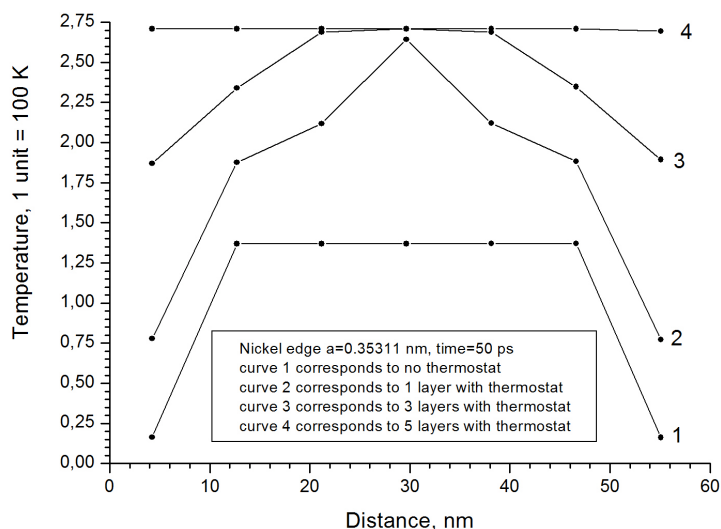
Fig. 2. Temperature distribution over the height of the sample

a parallel program was created. The developed program was carried out full-scale computational experiment whose purpose was to research the process of atoms thermodynamic equilibrium establishment in the sample heated to a predetermined temperature. Obtained in the calculation results demonstrated the adequacy of the proposed numerical approach to modern theoretical concepts of the simulated physical process. Comparing of the received results with the experiment was conducted on the basis of the known tabular data about the properties of nickel under normal conditions.

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