THE NUMERICAL STUDY OF PROPERTIES OF MAGNETIC MULTILAYER FILMS IN FRAME OF HEISENBERG MODEL BY HIGH PERFORMANCE COMPUTING

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Abstract: *the results of numerical calculations of the thermodynamic properties of multilayer films with alternating magnetic and non-magnetic layers were presented. Computer simulation of such structures within the frame of the classical Heisenberg model was carried out by Monte Carlo methods. For the Monte Carlo simulation, the Metropolis algorithm and its parallel implementation using MPI and the Wang-Landau algorithm were used. The thermodynamic characteristics of multilayer structures, such as the temperature behavior of magnetization, energy, and heat capacity, were studied.*
Keywords: *the Monte Carlo methods, Metropolis algorithm, Wang-Landau algorithm, Heisenberg model, multilayer structures.*

ЧИСЛЕННОЕ ИССЛЕДОВАНИЕ СВОЙСТВ МАГНИТНЫХ МНОГОСЛОЙНЫХ ПЛЕНОК В РАМКАХ МОДЕЛИ ГЕЙЗЕНБЕРГА С ПРИМЕНЕНИЕМ ВЫСОКОПРОИЗВОДИТЕЛЬНЫХ ВЫЧИСЛЕНИЙ

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Аннотация: *представлены результаты численных расчетов термодинамических свойств многослойных пленок с чередующимися магнитными и немагнитными слоями. Компьютерное моделирование таких структур в рамках классической модели Гейзенберга проводилось методами Монте-Карло. Для моделирования методом Монте-Карло использовался алгоритм Метрополиса и его параллельная реализация с использованием MPI, а также алгоритм Ванга-Ландау. Были изучены термодинамические характеристики многослойных структур, такие как температурное поведение намагниченности, энергии и теплоемкости.*
Ключевые слова: *методы Монте-Карло, алгоритм Метрополиса, алгоритм Ванга-Ландау, модель Гейзенберга, многослойные структуры.*

The necessity of studying magnetic multilayer structures is explained by the prospects of their practical application as a technological base for creating new storages medium [1, 2]. Multilayer structures are structures of

alternating magnetic and nonmagnetic layers. Within the frame of our model of the multilayer structure, the magnetic layer of the multilayer one has a size of $N \times N \times L$, and represents, the system of spins of Heisenberg placed in the nodes of a simple cubic lattice, in which the spin has up to 6 nearest neighbors in its film, as well as interact via the long-range direct exchange with all the spins belonging to the neighboring magnetic films. Non-magnetic layers reduce the energy, depending on their thickness. The Hamiltonian of the multilayers system was set as follows:

$$H = -J_1 \sum_{<i,j>} \vec{S}_i \vec{S}_j - J_{12} \sum_{<i,k>} \vec{S}_i \vec{S}_k - A_z \sum_i \vec{S}_i - h_z \sum_i \vec{S}_i , \qquad (1)$$

where $\vec{S}_i$ is the atomic spin at the i-th lattice site, J_1 – ferromagnetic short-range exchange interaction inside each layer, J_{12} – antiferromagnetic long-range exchange interaction between neighboring layers, $|A|$ - constant of magnetic anisotropy, h - external magnetic field.

The developed software is based on the new, promising programming language Rust. Rust supports functional, parallel (MPI), procedural and object-oriented programming, that is, almost the entire range of paradigms actually used in applied programming. For the Monte Carlo simulation, the Metropolis algorithm [3] and its parallel implementation using MPI and the Wang-Landau algorithm [4] were used.

The thermodynamic characteristics of multilayer structures, such as the temperature behavior of magnetization, energy, and heat capacity, were investigated using by the Monte Carlo methods, see Fig. 1.

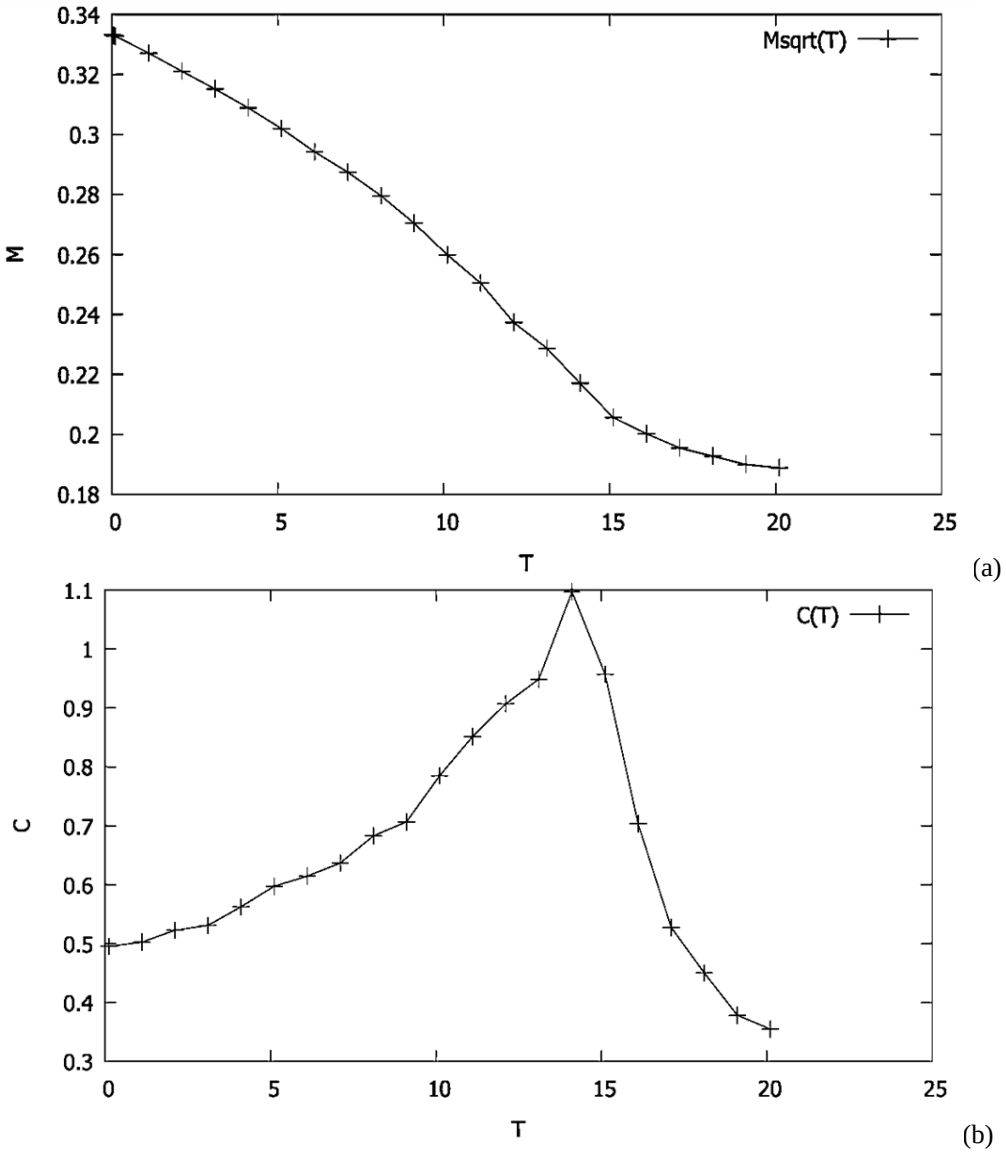

Fig. 1. The plots of temperature dependences for multilayer film: the quadratic magnetization (a), the energy (b)

In the frame of the classical Heisenberg model, lattice spin systems with direct short- and long-range exchange interactions were investigated by Monte Carlo methods. The thermodynamic properties of multilayer films with alternating magnetic and non-magnetic layers were studied.

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