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Manifestation of Slow Dynamics in Multilayer Nanostructures with Different Thicknesses of Magnetic Films

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Abstract. The results of a numerical Monte Carlo study of the behavior of a trilayer nanostructure with magnetization oriented in the film plane with ferromagnetic film thicknesses $N = 3$ and 21 MLs are presented. The non-equilibrium behavior of the structure has been investigated at the critical temperatures $T_c(N)$ and temperatures $T_c(N)/2$, $T_c(N)/4$, and the time dependence of the autocorrelation function during the evolution from different initial states and the dynamic susceptibility from the high-temperature initial state have been analyzed. Aging effects are revealed in the behavior of the two-temporal characteristics. The asymptotic values of the fluctuation-dissipative ratio for the structures with $N = 3$ and 21 MLs are calculated which indicate the violation of the fluctuation-dissipative theorem in the non-equilibrium behavior of these structures.

Keywords: Monte Carlo simulation, non-equilibrium behavior, anisotropic Heisenberg model, nanostructures, aging, fluctuation-dissipation ratio.

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The study of macroscopic statistical systems characterized by slow dynamics [1], as well as the study of the properties of ultrathin magnetic films [2] is currently of considerable interest. The increased interest in studying the behavior of ultrathin magnetic films is associated with the presence of unique their properties that differ significantly from those of bulk metals: sensitivity to the effects of anisotropy created by the crystal field of the substrate or nonmagnetic interlayers; the emergence of the effect of giant magnetoresistance; the manifestation of slow dynamics in a wider temperature range than in bulk materials.

It is known that multilayer magnetic structures are characterized by anomalously slow dynamics with the effects of aging and violation of the fluctuation-dissipative theorem predicted and observed in the slow evolution of systems from a non-equilibrium initial state [3, 4].

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The aim of this work is to simulate the non-equilibrium behavior of a trilayer nanostructure with different thicknesses of ferromagnetic films of $N = 3$ and 21 monolayers and magnetization oriented in the plane of the films.

1. Characteristics of non-equilibrium critical behaviour and results of simulations

The magnetic properties of ultrathin transition metal films in contact with nonmagnetic noble metal films are correctly described by the anisotropic Heisenberg model [5]:

$$\begin{aligned} H = &- J_1 \sum_{<i,j>}^{{N_s}^{(1,2)}} \left[{S_i}^x {S_j}^x + {S_i}^y {S_j}^y + (1 - \Delta(N)) {S_i}^z {S_j}^z \right] - \\ &- J_2 \sum_{<i \in N_1, j \in N_2>}^{L^2} \left[{S_i}^x {S_j}^x + {S_i}^y {S_j}^y + (1 - \Delta(N)) {S_i}^z {S_j}^z \right], \end{aligned} \qquad (1)$$

where S_i^x, S_i^y, S_i^z are components of the three-dimensional unit spin vector $\overrightarrow{S_i}$ in the sites of the fcc lattice of the trilayer structure Co/Cu/Co; ${N_s}^{(1,2)} = N \times L \times L$ is a number of spins in film 1 and 2 with $L = 64$ as linear size of the film; $\Delta(N)$ is dimensionless anisotropy parameter depending on the thickness of the ferromagnetic film, in this work $\Delta(N = 3) = 0.665$, $\Delta(N = 21) = 0.02$; $J_1 = 1$ is integral of the exchange interaction between spins inside the film, $J_2 = -0.1 J_1$ is the exchange integral of the interlayer interaction between spins on inner surface of films. The negativity of J_2 reflects the fact that the interlayer exchange interaction between the spins of ferromagnetic layers has an antiferromagnetic character with the magnetizations of neighboring layers oriented opposite to each other. The structure itself is schematically represented in Fig. 1.

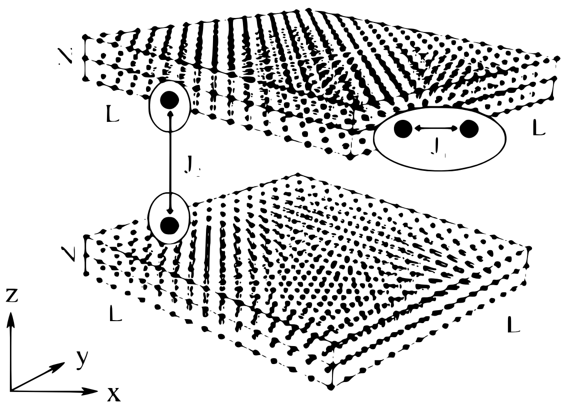

Fig. 1. Schematic representation of a multilayer nanostructure

The autocorrelation function $C(t, t_w)$ and the dynamical susceptibility $\chi(t, t_w)$ are considered as characteristics of nonequilibrium behavior:

- in this paper, the Metropolis algorithm was used to model the autocorrelation function

$$C(t,t_w) = \left\langle \frac{1}{N}\sum_{i=1}^{N} \overrightarrow{S}_i(t)\overrightarrow{S}_i(t_w)\right\rangle - \left\langle \frac{1}{N}\sum_{i=1}^{N} \overrightarrow{S}_i(t)\right\rangle \left\langle \frac{1}{N}\sum_{i=1}^{N} \overrightarrow{S}_i(t_w)\right\rangle; \qquad (2)$$

- the Glauber dynamics algorithm was used to model the dynamic susceptibility

$$\chi(t,t_w) = \frac{1}{T_c N}\sum_{i=1}^{N} \left\langle \overrightarrow{S}_i(t)\Delta\overrightarrow{S}_i(t_w)\right\rangle, \qquad (3)$$

$$\Delta\overrightarrow{S_i}(t_w) = \sum_{i=1}^{t_w} \overrightarrow{S_i}^{\parallel}\left(1 - \mathrm{th}\left(\frac{1}{2T_c}\Delta H_i(t)\right)\right). \qquad (4)$$

Statistical averaging, denoted in Eq. (2) and (3) by angle brackets, is implemented through averaging over runs with different initial states. Statistical averaging of the autocorrelation function $C(t,t_w)$ and dynamic susceptbility $\chi(t,t_w)$ was carried out on 3000 MC runs for every t_w.

In the course of this work, we numerically investigated the two-time dependence of the autocorrelation function $C(t,t_w)$ for different waiting times t_w during the evolution of the structure from different initial states at the critical temperature $T_c(N=3) = 2.3918(65)$ (Fig.2). The plots show that when evolving from the low-temperature completely ordered initial state with $m_0 = 1$, the autocorrelation function is characterized by a faster decline and weakening of the influence of the waiting time t_w than when evolving from the high-temperature initial state with $m_0 \ll 1$ for all quenching temperatures $T_s = T_c$, $T_c/2$, $T_c/4$. Aging effects are revealed which are manifested not only at the critical temperature T_c, but also in the whole low-temperature phase that is expressed in the slowing down of the time decay of $C(t,t_w)$ with increasing t_w.

It is also worth noting that the autocorrelation function in the evolution from the low-temperature completely ordered initial state with $m_0 = 1$ is characterized by a slower decline with increasing quenching temperature T_s that is opposite to the behavior of $C(t,t_w)$ in the evolution of the system from the high-temperature initial state, where the decline is faster with increasing T_s.

One of the issues considered in this work was the influence of the thickness of ferromagnetic films N on the behavior of the autocorrelation function $C(t,t_w)$ and dynamic susceptibility $\chi(t,t_w)$. Analysis of the time dependencies of these characteristics (Fig. 3) shows that the autocorrelation function $C(t,t_w)$ and the dynamic susceptibility $\chi(t,t_w)$ have a stronger dimensional dependence on N at critical temperatures $T_c(N=3) = 2.391(6)$, $T_c(N=21) = 3.21(3)$ than in the low-temperature phase with $T_s < T_c$.

The autocorrelation function $C(t,t_w)$ and the dynamic susceptibility $\chi(t,t_w)$ at the critical temperature $T_c(N)$ are found to decrease faster with increasing film thickness N. That is, the aging effects are weaken with increasing film thickness N. This is due to the weakening of the critical correlations at the dimensional transition in the structures from films with quasi two-dimensional properties for $N = 3$ ML to films with three-dimensional bulk properties for $N = 21$ ML.

At temperatures below the critical temperature, the opposite tendency of strengthening the effects of coalescence with increasing film thickness is observed. This is due to the increase in the characteristic correlation length of transverse spin correlations with decreasing temperature, leading to an increase in the correlation time and relaxation of the structure.

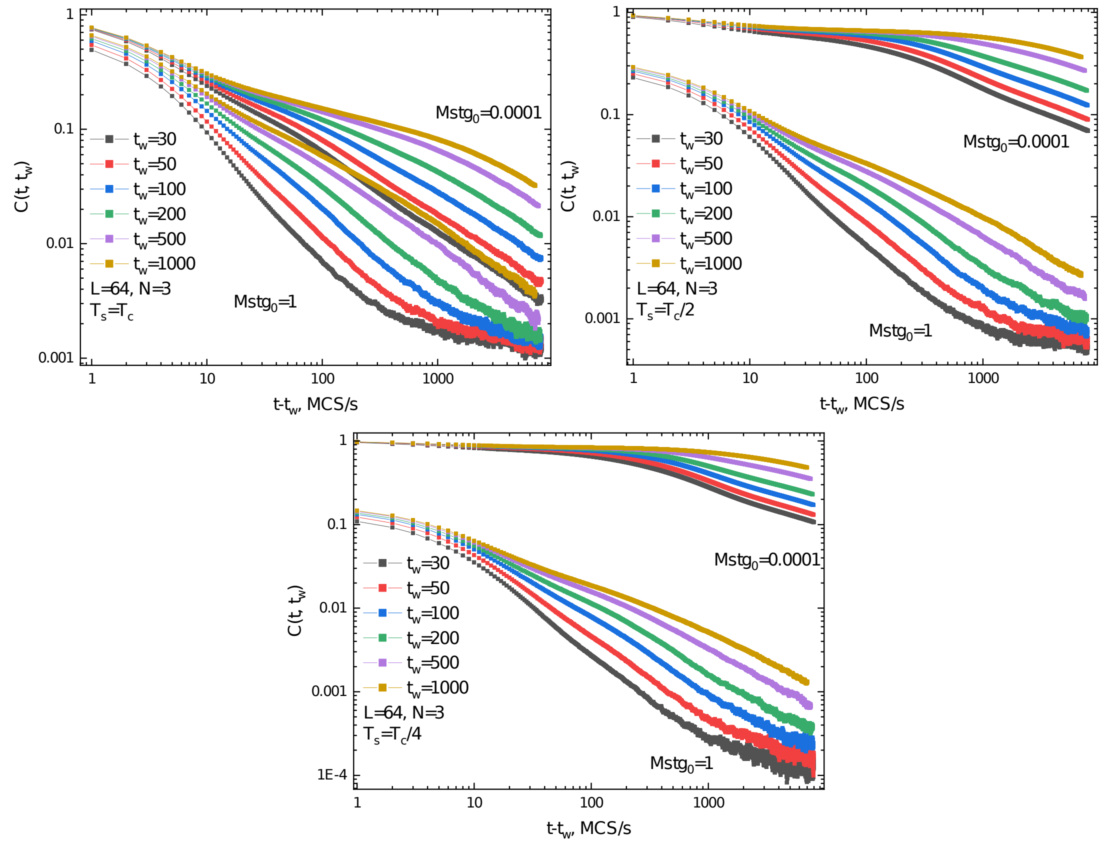

Fig. 2. Time dependence of $C(t, t_w)$ during the evolution of the structure with thickness $N = 3$ ML of ferromagnetic films from the low-temperature and high-temperature initial states for quenching temperatures $T_s = T_c$, $T_c/2$, $T_c/4$

For the first time, the calculation of the limiting fluctuation-dissipative ratio (FDR) X^∞ for multilayer nanostructures has been carried out. The FDR is an important universal characteristic of non-equilibrium processes in various systems with slow dynamics [6] and can be defined by the relation:

$$X^\infty = \lim_{t_w\to\infty} \lim_{t\to\infty} X(t, t_w) = \lim_{t_w\to\infty} \lim_{C\to\infty} T \frac{\partial\chi(t, t_w)}{\partial C(t, t_w)}. \tag{5}$$

Based on the calculated bivariate relationships for the autocorrelation function $C(t, t_w)$ and dynamic susceptibility $\chi(t, t_w)$ (Fig. 4), the asymptotic values of the FDR X^∞ were determined and presented in Tab. 1.

For structures with ferromagnetic film thicknesses $N = 3$ ML, the obtained asymptotic value of the FDR at the critical temperature T_c $X^\infty = 0.448(6)$ agrees very well with the value $X^\infty = 0.444(26)$ [7] for the 2d XY model at the Berezinskii–Kosterlitz–Towless phase transition temperature, and for structure with $N = 21$ ML $X^\infty = 0.385(4)$ agrees with the value $X^\infty = 0.383(6)$ [8] for the 3d isotropic Heisenberg model because of the small influence of anisotropy effects in these structures $(\Delta(N = 21) = 0.02)$.

For temperatures $T_s < T_c$, the asymptotic values of the FDR exhibit much larger values than at the critical temperature T_c.

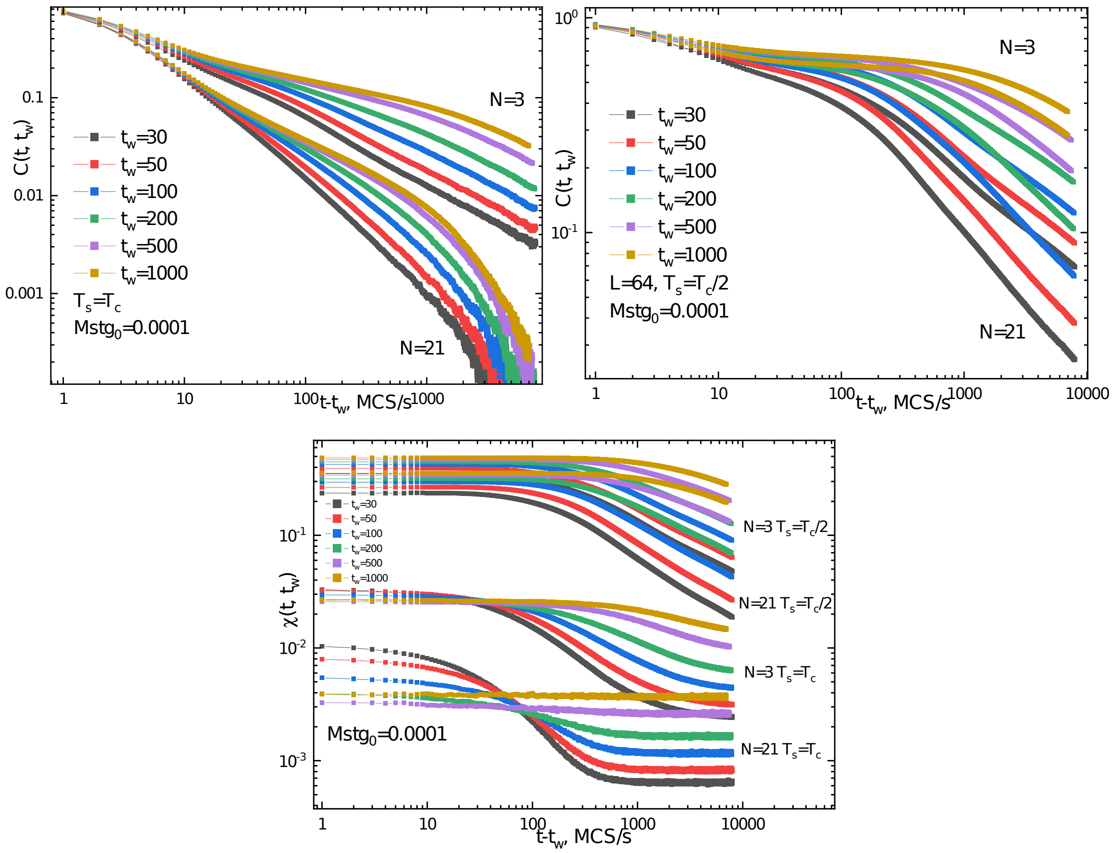

Fig. 3. Time dependence of $C(t, t_w)$ and $\chi(t, t_w)$ during the evolution of the structures from the high-temperature initial state for film thicknesses $N = 3$, 21 ML at quenching temperatures $T_s = T_c$ and $T_s = T_c/2$

Table 1. Asymptotical values of the FDR for different quenching temperatures T_s and film thicknesses $N = 3$ and 21 ML

T_s	$T_c(N)$	$T_c(N)/2$	$T_c(N)/4$
$X^\infty(N = 3)$	0.448(6)	0.909(1)	0.9672(7)
$X^\infty(N = 21)$	0.385(4)	0.850(1)	0.921(7)

Conclusions

In conclusion, we note that in the presented work we have carried out a numerical Monte Carlo study of the manifestation of slow dynamics features in the magnetic properties of a multilayer nanostructure consisting of two ferromagnetic films with thicknesses N = 3, 21 ML, separated by a film of nonmagnetic metal and connected by an antiferromagnetic exchange interaction. The anisotropic Heisenberg model with anisotropy of the "easy" plane type was applied to describe the properties of such a structure. The non-equilibrium behavior of the structures has been investigated not only at the critical temperature but also in the whole low-temperature phase. The aging effects have been revealed in the time dependence of the autocorrelation function and the dynamic susceptibility. The calculation of the limiting fluctuation-dissipative ratios

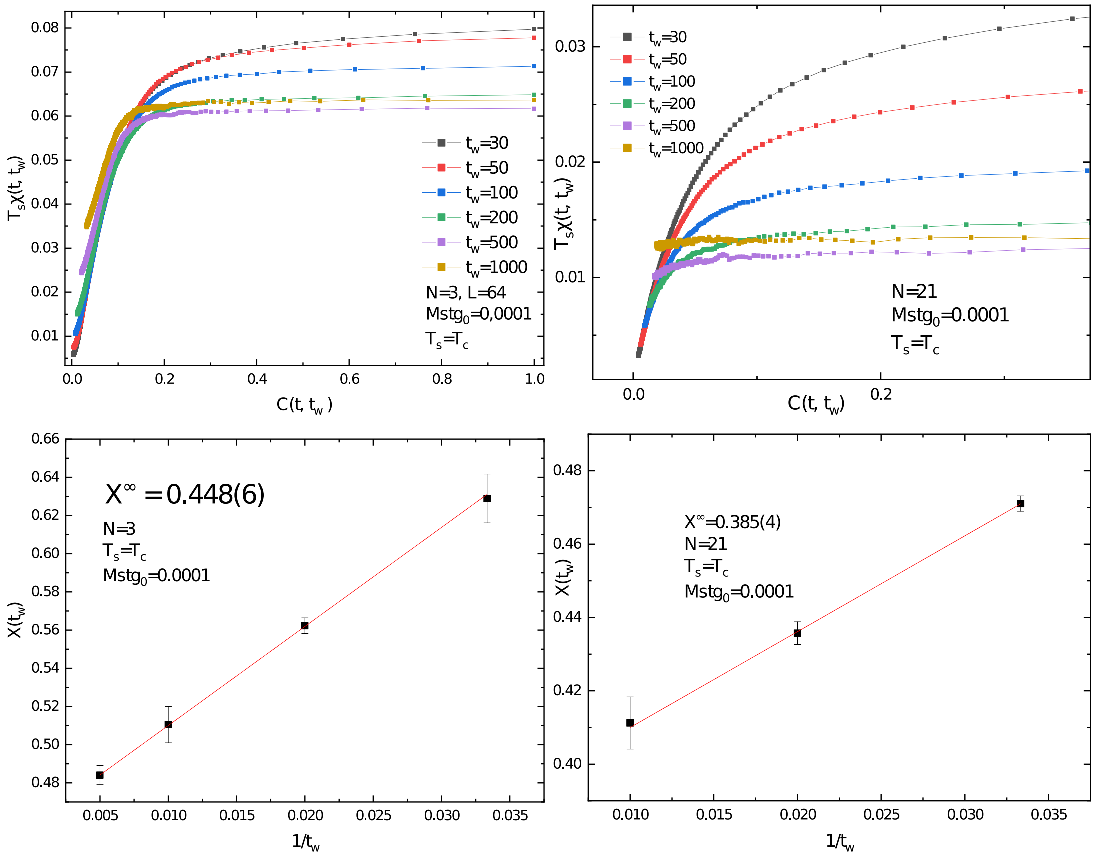

Fig. 4. Parametric dependence of $T_c\chi(t, t_w)$ on $C(t, t_w)$ and linear approximation of the FDR $X(t_w \to \infty)$ for different t_w to determine X^∞ for a film with $N = 3, 21$ at $T_s = T_c$

$X^\infty(N = 3, T_c) = 0.448(6)$ and $X^\infty(N = 21, T_c) = 0.383(6)$ for the case of structure evolution from the high-temperature initial state has been carried out. The obtained values of the FDR at the critical temperatures demonstrate the dimensional changes in non-equilibrium behavior of structures from quasi two-dimensional properties for $N = 3$ ML to three-dimensional bulk properties for $N = 21$ ML. It is revealed that the asymptotical values of the FDR lead to unity as the quenching temperature with $T_s < T_c(N)$ decreases, indicating a tendency for the non-equilibrium effects to decrease.

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References

[1] M.Henkel, M.Pleimling, Non-Equilibrium Phase Transitions, vol. 2: Ageing and Dynamical Scaling far from Equilibrium (Theoretical and Mathematical Physics), Springer, 2010.

[2] C.A.F.Vaz, J.A.C.Bland, G.Lauhoff, Magnetism in ultrathis film structures, *Rep. Prog. Phys.*, **71**(2008), 056501. DOI:10.1088/0034-4885/71/5/056501

[3] T.Mukherjee, M.Pleimling, Ch.Binek, Probing equilibrium by nonequilibrium dynamics: aging in Co/Cr superlattices, *Phys. Rev. B*, **82**(2010), 134425.
DOI: 10.1103/PhysRevB.82.134425

[4] V.V.Prudnikov, P.V.Prudnikov, A.N.Purtov, M.V.Mamonova, Aging effects in the nonequilibrium behavior of multilayer magnetic superstructures, *JETP Lett.*, **107**(2016), no. 9, 569–576.

[5] V.V.Prudnikov, P.V.Prudnikov, M.V.Mamonova, Problems of Modern Natural Science, Omsk: Publishing house of Omsk State University, 2019 (in Russian).

[6] V.V.Prudnikov, P.V.Prudnikov, M.V.Mamonova, Nonequilibrium critical behavior of model statistical systems and methods for the description of its features, *Physics–Uspekhi*, **60**(2017), no. 8, 762–797. DOI: 10.3367/ufne.2017.02.038067

[7] P.V.Prudnikov, V.V.Prudnikov, I.S.Popov, Non-equilibrium aging effects in the critical behavior of structurally disordered planar magnetics, *JETP Letters*, **101**(2015), no. 8, 539–544.
DOI: 10.1134/S0021364015080135

[8] V.V.Prudnikov, P.V.Prudnikov, E.A.Pospelov, A.S.Lyakh, Simulation of non-equilibrium critical behavior of the 3D isotropic and anisotropic Heisenderg models, *Journal of Physics: Conf. Ser.*, **1740**(2021), 012004. DOI: 10.1088/1742-6596/1740/1/012004

Проявление медленной динамики в мультислойных наноструктурах с различными толщинами магнитных пленок

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Аннотация. Представлены результаты численного Монте-Карло исследования поведения трехслойной наноструктуры с толщиной ферромагнитной пленки $N = 3$ и 21 МС и намагниченностью, ориентированной в плоскости пленки. Исследовано неравновесное поведение структуры при критических температурах $T_c(N)$ и температурах $T_c(N)/2$, $T_c(N)/4$, а также временная зависимость автокорреляционной функции при эволюции системы из различных начальных состояний и динамической восприимчивости при эволюции из высокотемпературного начального состояния. Эффекты старения проявляются в поведении двухвременных характеристик. Рассчитаны асимптотические значения флуктуационно-диссипативного отношения для структур с $N = 3$ и 21 МС, которые указывают на нарушение флуктуационно-диссипативной теоремы при неравновесном поведении этих структур.

Ключевые слова: метод Монте-Карло, неравновесное критическое поведение, анизотропная модель Гейзенберга, наноструктуры, эффекты старения, флуктуационно-диссипативное отношение.