Programmable magnetic domain evolution in magnetic auxetic systems

K. K. Dudek¹, W. Wolak², M. R. Dudek*², R. Caruana-Gauci¹, R. Gatt¹, K. W. Wojciechowski³, and J. N. Grima¹,⁴

¹ Metamaterials Unit, Faculty of Science, University of Malta, Msida MSD 2080, Malta
² Institute of Physics, University of Zielona Gora, ul. Szafrana 4a, 65-069 Zielona Gora, Poland
³ Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, 60-179 Poznan, Poland
⁴ Department of Chemistry, Faculty of Science, University of Malta, Msida MSD 2080, Malta

Received 20 April 2017, revised 23 June 2017, accepted 6 July 2017
Published online 14 July 2017

Keywords auxetic, Ising model, magnetic domains, mechanical metamaterials

* Corresponding author: e-mail m.dudek@if.uz.zgora.pl, Phone: +48 68 328 2910, Fax: +48 68 328 2920

In this work, we investigate the evolution of magnetic domains with time in magnetic auxetic systems using the Ising model. We show that the mechanical deformation of the structure affects the way how domains evolve and that their rate of growth does not follow a well-known power law associated with the Ising model for systems corresponding to a specific distance between Ising spins. We also show that the variation in the rate of deformation of the system leads to completely different results in terms of the change in size of magnetic domains and domain energy. This means that upon changing the speed used to deform the system, it is possible to control the growth of magnetic domains and hence control the magnetic properties of the whole system. This may prove to be very important in the case of potential applications such as magnetic freezers where the magnetocaloric effect resulting with a change in temperature could be affected by the rate of deformation of the discussed auxetic structure.

1 Introduction Over the years, the Ising model [1] has been proven to be a great tool in order to investigate a wide range of physical phenomena. In particular, based on the famous Onsager solution [2, 3] for the two-dimensional square lattice at zero magnetic field, this model allowed to gain a fundamental understanding of critical phenomena. It also led to numerous discoveries in areas such as social physics [4], modelling of neural networks [5] and economy [6]. The interest of scientists in this particular technique resulted with numerous studies in which it was shown that in the systems modelled with the Ising model, the mean size of magnetic domain (after a temperature quench of the system from a disordered to an ordered phase) increases in time accordingly to a particular power law. More specifically, it changes proportionally to the evolution time raised to the power of 1/2 or 1/3 for systems with a non-conserved [7, 8] or conserved [9, 10] order parameter respectively. A detailed mathematical description of different laws governing a domain growth in various systems can be found in papers by Bray [11] and Rutenberg [12]. At this point, it is important to note that the results discussed above were obtained for systems in which the distances between the neighbouring spins within the system were fixed. These rules regarding the rate of growth of domains in magnetic systems do not have to apply to systems in which the distances between the neighbouring spins change in time. In fact, over the years, numerous attempts [13–15] have been made to analyse various physical phenomena associated with the deformed Ising models (e.g., compressed) with one of the most promising studies being the work of Cirillo et al. [16] where it was shown that the above characteristics are not valid for the Ising model subjected to a shear flow. This also suggests that if one was to be able to control the distance between the neighbouring Ising spins then it might be possible to observe a completely new type of evolution of magnetic domains in time.

Mechanical metamaterials (i.e., systems which attain unusual mechanical properties due to their structure rather than their chemical composition), is a class of systems which may exhibit unusual behaviour upon being subjected to a mechanical deformation, that is the structure expands in
the transverse direction when uniaxially stretched (negative Poisson’s ratio) [17–26] which behaviour is often referred to as auxetic behaviour [21]. These systems may be used to conveniently change the distance between the elements constituting the structure in a rather unusual pattern which would not be possible for conventional systems. Some of the most studied mechanical metamaterials are rotating rigid unit systems [27–29] with one of the prime examples being ‘rotating squares system’ [30] with a Poisson’s ratio of −1. This particular system deforms in a highly symmetric manner which permits specific distances within the model, for example the distances between the centres of all of the neighbouring units, to change by exactly the same amount. This in turn makes this system to be a perfect candidate to alter the geometry of the Ising model throughout the process of simulation.

At this point, it is important to note that even though in general one could consider an arbitrary mechanical system in order to change the distance between the neighbouring spins, the choice of the system of rotating square units is associated with the fact that in the case of this model, at each stage of the deformation process, positions of centres of respective units may be represented by a square lattice. This in turn makes it possible to use the analytical Onsager solution [2] for the Ising model defined on a square lattice, in which case the exact value of the critical temperature is known. This would not be possible in the case of an arbitrary lattice as the analytical solution concerning the value of the critical temperature in the system comprised of Ising spins is known only for a very limited number of lattices. In view of this, such temperature would have to be determined numerically by means of the appropriate computer simulation.

2 Model In this work, the two-dimensional model based on a set of \( N_x \times N_y \) rigid squares connected at vertices is going to be discussed (see Fig. 1). It is assumed that each square has a side length of \( a \). The angle between the adjacent units is denoted as \( 2\theta \) and due to geometric constraints its value lies within the interval between 0° and 180°. Furthermore, in order to analyse the evolution of magnetic domains in time in such system, it is assumed that located at the centre of each square there is an Ising spin (see Fig. 1). These spins assume one of the two possible orientations, that is either ‘up’ or ‘down’ which states correspond to values 1 and −1 respectively. One may note that Ising spins in such system form a square lattice with the distance \( d \) separating each pair of neighbouring spins which also means that \( d \) stands for a distance between the centres of adjacent squares.

At this point, it is important to highlight the fact that even though in the case of this work only the theoretical model is being discussed, one could potentially consider an experimental realisation of this model. More specifically, it is possible to consider the investigated system as a nonmagnetic mechanical structure with magnetic nanoparticles located at the centre of each of the rigid units.

Evolution of magnetic domains (collection of spins having the same orientation) is going to be investigated through the use of the well-known Metropolis algorithm [31] (with periodic boundary conditions imposed on the discussed system) in which case the energy of interaction between the neighbouring spins may be defined with the help of the nearest-neighbour Ising model Hamiltonian \( H \) in the following manner:

\[
H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad (1)
\]

where \( J \) is the coupling constant, the angular brackets denote summation over the \( N_p \) nearest-neighbour square centre pairs with Ising spins \( \sigma_i \) and \( \sigma_j \). The value of \( J \) depends on a distance \( d \) as shown in the following equation: \( J = J_0/d^3 \) [32], which expression was used recently for modelling of the magnetocaloric effect in magneto-auxetic metamaterials [33]. At this point one may also note that the value of \( d \) depends on the extent of the angle \( 2\theta \) and may be expressed as follows:

\[
d = a \sqrt{2} \sin\left(\frac{\pi}{4} + \theta\right). \quad (2)
\]

It means that the energy of interaction between the adjacent magnetic moments changes according to the value of the angle \( \theta \). It also means that the critical temperature \( T_c \) changes with the value of \( \theta \) which stems from the fact that this particular quantity depends on \( J \) = \( J(\theta) \). The value of \( T_c \) is given by [33]:

\[
T_c(\theta) = \frac{2.269 J_0}{k_B} \left( a \sqrt{2} \sin\left(\frac{\pi}{4} + \theta\right) \right)^{-3}, \quad (3)
\]
where \( k_B \) denotes the Boltzmann constant. In order to ensure that the initial state of the system resembles the situation which one would expect in reality, the fully-closed system (2\( \theta = 0^\circ \)) is initially subjected to the relatively high temperature \( T_h \) (significantly above the value of \( T_c(\theta) \)) for a duration of \( N_{\text{initial}} \) Monte Carlo steps. After this pre-heating procedure, the evolution of magnetic domains in the system is investigated in the case of a deformation process corresponding to the change in the value of 2\( \theta \) angle from 0\(^\circ\) to 180\(^\circ\) at a certain temperature \( T \). At this point, one should note that a change in the value of the angle 2\( \theta \) from 0\(^\circ\) to 90\(^\circ\) (maximal distance between adjacent spins) corresponds to an increase in the distance between the neighbouring spins by 41% which is associated with a significant change in the magnitude of \( J \).

As mentioned before, the Ising spins defined in this work are considered to represent magnetic nanoparticles embedded within the discussed nonmagnetic system. In the case of a number of experimental studies, it was shown that dense ensembles of magnetic nanoparticles can exhibit a collective behaviour which is typical for spin-glass or superferromagnetic systems. As the matter of fact, there are theoretical studies where the evolution of magnetic domains was investigated in the case of systems analogous to the one mentioned above [34]. In such systems, each of the magnetic nanoparticles (above the blocking temperature) acts as a single superspin interacting with the surrounding superspins through dipolar interactions [35]. These interactions may result with spin reorientation which process is governed by the Nel relaxation mechanism.

3 Results and discussion
In order to analyse the evolution of magnetic domains, the discussed system was mechanically deformed at a temperature of \( T = 77.35K \) with the angle 2\( \theta \) being changed from 0\(^\circ\) to 180\(^\circ\). The value of \( T \) was chosen in a way which, for different values of \( \theta \), results with it being both greater and lower than the value of \( T_c \) (see Eq. (3)) throughout the deformation process. More specifically, the value of \( T/T_c \) is equal to 2.142 and 0.963 in the case of 2\( \theta \) assuming the value of 0\(^\circ\) and 90\(^\circ\) respectively. The process of deformation of the discussed system was investigated for different rates of opening of the angle 2\( \theta \), that is \( \omega = \{0.5, 1.0, 10, 100\}^\circ/\text{MCs} \) (\(^\circ/\text{MCs} \) – degree per Monte Carlo step). The remaining parameters defined in the Model section were set to be the following: \( N_x \times N_y = 500 \times 500, a = 18.5 \text{ nm}, T_h = 800 \text{ K}, N_{\text{initial}} = 5 \) and \( J_0 = 50.42 \text{ eV nm}^3 \). One can note that the linear dimension corresponding to the square-like unit, that is dimension \( a \), was set in a way so that there is enough space for insertion of a single-domain magnetic nanoparticle which in this study is represented by the Ising spin. Such magnetic nanoparticles may vary in size but usually they do not exceed the size of 15 nm. At this point it is also worth to note that before the pre-heating procedure, which took place before the beginning of the deformation, the orientation of spins within the system was selected randomly. Furthermore, in order to ensure high quality of the generated results, each set of results was averaged 10 times.

Based on Fig. 2(a), one can note that throughout the process of mechanical deformation, the change in size of magnetic domains (represented by means of the correlation length \( r \)) does not follow the well-known power law corresponding to Ising systems with a non-conserved order parameter, that is is not proportional to the time raised to the power of 1/2. Instead, the correlation length (it is an average distance from an arbitrary spin to a boundary of a domain at which it is located) of the deformed system exhibits a more complex behaviour with two local extrema being observed. More specifically, at the range of 2\( \theta \) between 0\(^\circ\) and 30\(^\circ\) the value of \( r \) increases in order to subsequently start decreasing upon surpassing the configuration corresponding to 2\( \theta = 30^\circ \). This trend is continued up to the point where the local minimum of \( r \) is reached, that is around 90\(^\circ\) – 100\(^\circ\). During the remaining part of the mechanical deformation of the discussed system the angle 2\( \theta \) is being changed from 90\(^\circ\) to 180\(^\circ\) (this process corresponds to a decrease of the distance between the adjacent spins) which results with an increase of the magnitude of the correlation length. This novel behaviour can be easily understood if one was to analyse the evolution of magnetic domains in time in the case of the analogous system in which the distance between the adjacent units does not change throughout the simulation, that is \( \theta = \text{const.} \) (see Fig. 2(b)). In this case, after generating results for a number of systems corresponding to a fixed value of \( \theta \), it is possible to imagine the situation where as time is increasing, one moves from the graph corresponding to the system associated with a constant value of 2\( \theta = 0^\circ \) to 2\( \theta = 90^\circ \) and then back from 90\(^\circ\) to 0\(^\circ\). Should one assume that a transition between different lines occurs always after a particular time step \( \Delta t \) (in the case of the example shown in Fig. 2(b) \( \Delta t = 10 \) MCs), then it would be possible to connect the consecutive points on different graphs in order to obtain the domain evolution represented by means of the black dashed line (see Fig. 2(b)). One may note that this line closely resembles the type of the domain evolution observed for a system subjected to a deformation process, which process corresponds to \( \omega = 1^\circ/\text{MCs} \) in the case of the provided example. Furthermore, in the case of Fig. 2(b), the plots associated with relatively small values of \( \theta \) correspond to the situation where \( T < T_c \). In such cases the emergence of the formerly discussed power law is expected (\( r \propto t^\alpha \)), which trend may be easily observed taking the system corresponding to 2\( \theta = 0^\circ \) as an example. In this particular case, the exponent \( \alpha \) associated with the system is equal to 0.49913 ± 0.00098.

It is also worth to mention that the only mechanism governing the domain growth in the system corresponding both to a fixed and changing value of \( \theta \), is the competition between ordering and dissipation. A potential deformation of the lattice with Ising spins only affects the magnitude of
their interaction and does not prevent the occurrence of domain evolution.

Another interesting result corresponds to the effect which the rate of opening of the angle 2θ has on the evolution of magnetic domains in the discussed system. As shown in Fig. 2(a), a variation in the magnitude of the angular velocity ω allows to control the growth of domains within the system. In particular, it may be noted that the lower the magnitude of ω, the larger the value of r. Based on Fig. 2(a) one can also see that there is a certain threshold value of ω below which value the system does exhibit the characteristics described above. In the case of results presented in Fig. 2(a) such threshold value would may be found in the vicinity of ω = 10°/MCs. Above this value,
magnetic domains do not have enough time to evolve during the deformation process which leads to significantly lower values of $r$. Moreover, in the case of relatively high values of $\omega$, the local minimum of the function of $r$, which might be observed in the vicinity of $90^\circ$, disappears. A clear difference between the evolution of domain in systems deformed with relatively high and relatively low value of $\omega$ is visualised in Fig. 3.

It is also possible to analyse the domain boundary energy $E$ during the deformation of the discussed system. This energy is calculated as a sum of energies of all pairs of spins within the system which have opposite orientation and are located on the opposite sides of the boundary separating any two domains. Based on Fig. 4, one can note that the change in $\omega$ results with qualitatively different results in terms of the energy $E$ for systems corresponding to relatively large and small values of $\omega$. This stems from the fact that the energy $E$ depends on the total length of boundaries within the system, which quantity changes depending on the value of $\omega$.

All of this is very important as it is shown that it is possible to control the evolution of domains upon changing the magnitude of the angular velocity $\omega$. It is also shown that the variation in the value of $\omega$ leads to very different results in terms of the energy $E$. This control over the change in the value of the energy throughout the process of deformation may be used in order to control the magnitude of the mechanically-driven magnetocaloric effect as shown by Dudek et al. [33]. This in turn would allow to increase or decrease the value of temperature of the system in a controllable manner without the presence of the external magnetic field. This result could prove to be very important for scientists working on novel techniques associated with magnetic refrigeration particularly in view of the recent wide interest in magnetic metamaterials and other systems [36–41]. It is also hoped that this work may contribute to the further discussion concerning the use of the Ising model in the case of hierarchical systems [42–44] which could possibly lead to novel applications of such systems.

4 Conclusions In conclusion, in this work it was shown that the evolution of magnetic domains in the Ising model associated with the magnetic system of rotating squares does not follow a well-known power law which is valid for systems in which the distance between the neighbouring units remains constant throughout the simulation. It was also shown that the evolution of magnetic domains can be controlled upon altering the magnitude of the angular velocity of rigid units constituting the system. Another result obtained through this study shows that upon changing the value of the angular velocity of rigid units it is possible to control the energy of the system. This in turn may be used in order to control the magnitude of the mechanically-driven magnetocaloric effect which phenomenon can be used to alter the temperature of the system. This result could prove to be useful in the case of applications related to magnetic refrigeration.

References