

Research Article

Possibility of Phase Transition in Mechanical Metamaterials

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Abstract:

Based on the available knowledge from numerous simulation studies regarding the occurrence of metamaterial phase transition, structures were produced that exhibit a real auxetic-non-auxetic transition. The occurrence of this transition was possible thanks to the modified structure of rotating rectangles, showing significant dimensional changes. Through analysis and experimental evidence, it has been shown that there are limiting values of parameters, above which the Poisson's ratio becomes positive, and the structure loses its auxetic properties. It has been demonstrated that through the stretching of such structures, with a gradually increasing linear elongation horizontally, there is a curvilinear increase in elongation vertically. For rectangular unit cells with a parameter $a/b > 1.5$ and $x = 0.1$, the relationship between elongation in the horizontal and vertical directions ($\Delta X_2/X_2 = f(\Delta X_1/X_1)$) has a maximum and a zero point ($\Delta X_2/X_2 = 0$), which corresponds to the occurrence of a phase transition. The Poisson's ratio in this area ranges from $-\infty$ to $+\infty$. Such a huge auxetic effect can be achieved through the anisotropy of the structure. In the phase diagram, the Poisson's ratio – degree of deformation shows a specific area corresponding to a sudden transition in auxetic properties, where it concerns a phase transition without changes in symmetry. Morphologically, instead of two phases, there is only one with the same spatial arrangement of unit cells, differing only in linear dimensions.

Keywords: Mechanical Metamaterials, Auxetics, Phase Transition.

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INTRODUCTION

A mechanical metamaterial is a type of artificial structure built from unit cells with properties that contradict the properties of natural materials encountered every day. When subjected to an external force, the material deforms, expanding vertically and horizontally when stretched and contracting uniformly when compressed. Such reactions of structures to loads can lead to negative Poisson's ratio values, which is referred to as auxetic behavior. Depending on the type of unit cells and the arrangement of the structure, this behavior may involve a change in its dimensions to the point where it loses its auxetic properties.

The shifting of the structure under load involves the transmission of a mechanical stimulus between the unit cells, whereas they must exhibit adequate stiffness so that their connections allow for their movement through flexibility.

The functionality of such materials is limited by their tolerance to damage and defects, better known as 'resistance to cracking.' The poor tolerance for damage and defects mainly applies to unit cell connections. Such structures have a high probability of getting damaged due to critical stresses generated at the joints.

Given the possibility of changes in the properties of metamaterial structures and the occurrence of auxetic and non-auxetic phases, it can lead to the occurrence of a phase transition. A hypothetical metamaterial phase transition would become part of the large family of phase transitions in the solid phase.

In general, phase transitions are special phenomena associated with a sudden change in physical properties as a result of a gradual change in one of the parameters. Another definition states that a phase transition is a change in the macrostate of a set of interacting structural elements caused by a change in the external conditions, more precisely in the control parameter, such as temperature, pressure, magnetic field, or mechanical interactions. It should be added that a phase transition is a change in the nature of the phases or their number as a result of changes in the mentioned external conditions.

According to Ehrenfest, based on thermodynamic analysis, phase transitions can be classified into first-

and second-order transitions, separating material states with different properties. First-order transitions – associated with the emission or absorption of heat – are characterized by the appearance of discontinuities in thermodynamic quantities. This means that at the transition temperature in type I phase transitions, there is an increase in enthalpy, entropy, and density. Ehrenfest's second-order transitions involve continuity regarding changes in specific heat, magnetic susceptibility, and the thermal expansion coefficient.

This classification of phase transitions indicates that the transition point corresponds to a specific temperature T_{trans} , with a continuous change in temperature leading to the occurrence of a phase transition. When it comes to solid-state transitions, the first-order ones include allotropic and polymorphic transitions, superconducting phase – non-superconducting phase transition (in a magnetic field), martensitic transition, and order-disorder transition, as well as ferromagnet – paraelectric transition. The first two transitions (allotropic and polymorphic) are triggered by a change in temperature; the superconducting transition is triggered by a change in temperature and magnetic field intensity, while the martensitic transition is triggered by a change in temperature and the mechanical stimulus. The martensitic transition is a polymorphic phase transition that occurs in a certain temperature range and involves a regular modification of the crystal lattice. The transition onset is triggered by mechanical stress, and a temperature gradient is necessary for its progression. An internal structural change occurs in the process, defined as the transition from austenite to martensite and vice versa.

The mentioned examples of phase transition involve the change from one material phase into another caused by changes in temperature, pressure, stress, or chemical interactions. The change may involve one or several phases that transform into another phase or a mixture of phases since the initial state is less stable than the final one. From a thermodynamic point of view, it can be stated that at the transition temperature T_{trans} , both phases remain in equilibrium, i.e., in the well-known examples of phase transitions, it is almost always possible to distinguish two different structural solid phases. Exceptions include specific phase transitions

that do not involve internal structural changes, such as the superconducting phase – non-superconducting phase transition (in a magnetic field) and the auxetic – non-auxetic transition. This indicates that there is no equilibrium of the two phases at the transition point. Structurally, it is the same phase whose properties change with the changing conditions.

In the case of metamaterial phase transition through linear dimensional changes (tension or compression), the Poisson's ratio changes from negative to positive values (Grima 2004). The transition is accompanied by a change in from auxetic to non-auxetic properties (the sign of the Poisson's ratio changing from positive to negative). The two phases do not differ in the spatial arrangement of unit cells but exhibit different behavior only due to their different linear dimensions. Unlike the hitherto known phase transitions, the two phases cannot occur simultaneously, i.e., there is no equilibrium state between the auxetic phase and the non-auxetic phase (Wang, L, 2022).

The present work demonstrates the phase transition from auxetic to non-auxetic phase, both through the analysis of the behavior of a selected metamaterial structure as well as through experimental studies of the assembled structure of rotating rectangles.

IMPLEMENTATION OF THE AUXETIC-NONAUXETIC TRANSITION

Examples of mechanical metamaterials have been identified in which an auxetic-nonauxetic transformation is feasible. This requires a suitably large change in the structure's linear dimensions, which is unattainable for the already-known metamaterial structures. All these structures are usually compliant mechanisms (monolithic structures), in which

changes in linear dimensions are limited by the elastic properties of the unit cell connections, resulting in minimal changes in dimensions under load.

Such restrictions do not apply to the so-called modified structure of rotating rectangles (Plewa, 2024).

The concept of modifying two-dimensional rotating rectangles was based on the fact that the rectangular unit cells are connected by pivots at their corners, and the overlapping unit cells exhibit slight friction (depending on the degree of roughness). A prerequisite for the proper functioning of the structure is the rigidity of the material of the rectangular units, which interact with each other through pivot points in tension or compression. In the closed system, however, parts of the edges of the rigid rectangles rest on each other and exhibit resistance in tension. When the system is being stretched, the rectangular unit cells connected by pivots not only rotate relative to each other but also undergo translation. For such an anisotropic material, the change in its dimensions depends on the direction of stretching.

The modified structure of rotating rectangles (checkerboard-type) presented in Figure 1 is an example of a well-functioning auxetic structure resistant to cracking and other kinds of damage. Depending on the parameters of unit cells, the changes in its dimensions can reach values of up to <40% (Plewa, 2024).

Metamaterials are composed of rotating rigid units in which internal voids allow the units to rotate freely and shift under loading conditions. The presented structures are anisotropic, which leads to different dimensional changes under loading.

In Figure 1, it can be seen that stretching the structure horizontally increases size X1 continuously, whereas

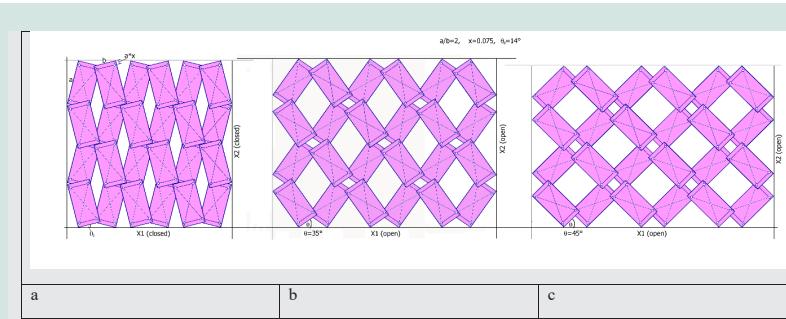


Figure 1: Example structure of rotating rectangles in the *closed* system (a) and in the *open* systems (b) and (c) with marked linear dimensions and unit cell parameters.

the vertical size X_2 first increases and then decreases. This has consequences for the value of the Poisson's ratio, which transitions from negative values to positive values.

The dimensional changes are used to calculate the Poisson's ratio, defined as a dimensionless constant of anisotropic material, expressed as the ratio of negative relative transverse strain $\Delta X_1/X_1 = \varepsilon_x$ to the relative longitudinal strain $\Delta X_2/X_2 = \varepsilon_y$ of the material under load.

$$\nu = -\varepsilon_x / \varepsilon_y \quad (1)$$

Where ε_x lateral strain and ε_y longitudinal strain

For elastomeric materials, tensile strain leads to bidirectional expansion, while compressive strain causes bidirectional contraction.

Poisson's ratio for such structures can be adjusted by modifying the geometric parameters a/b and x . Considering three different rectangular unit cell geometries, it is possible to determine the changes in the Poisson's ratio, along with elongation, when stretching the structures from the *closed* to the *open* system. This indicates that the phase transition is induced through motion.

Figure 2 shows the change in the Poisson's ratio as a function of elongation for the given geometric parameters a/b and x . A particular thing to note in the diagrams is that for elongated rectangular unit cells, there is a sudden change in Poisson's ratio value for specific values of elongation. For the parameters $a/b=1.5$ and $x=0.1$, the structure exhibits auxetic behavior across the entire elongation range, while for parameters $a/b=2$ and 2.5 , it exhibits partial auxetic behavior – only

for lower elongation values.

In the phase diagram, the Poisson's ratio – the degree of deformation shows a particular point corresponding to a sudden transition in the auxetic properties, although the symmetry of the structure is retained, meaning that this is a phase transition without changes in symmetry.

It is typical in this case that for increasing deformation, the negative value of the Poisson's ratio increases.

With the horizontal expansion $\Delta X_1/X_1$, the vertical expansion $\Delta X_2/X_2$ also increases monotonically. This tendency is present in structures with the geometric parameter $a/b < 1.5$. However, for a structure formed from rectangular unit cells with parameters $a/b=2$ and 2.5 , there is an unusual effect of local reduction in vertical expansion while there is a continuous increase in horizontal expansion. The structure initially increases its dimensions as it is stretched (uniaxially), utilizing the homogeneity of rigid units and practically demonstrating reliability for any number of elements, and then, upon further stretching, it slightly contracts. In structures of this kind, there may be a critical moment at which the Poisson's ratio changes its sign depending on the degree of deformation, which can be considered a phase transition between an auxetic and non-auxetic phase.

It can be demonstrated that there are parameter limit values above which the Poisson's ratio becomes positive and the structure loses its auxetic properties. For longer rectangles (structures with $a/b=2.5$ – Figure 2), extremely high negative Poisson's ratio values are obtained, but only for small opening angles of the

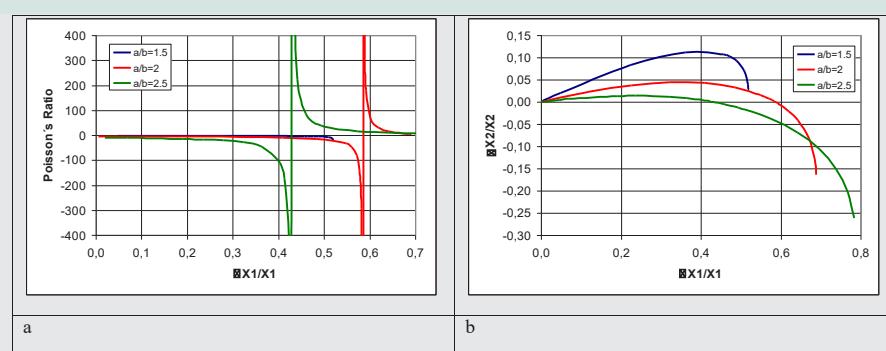


Figure 2: Change in the Poisson's ratio as a function of elongation for the structure of modified rotating rectangles in tension –a, and the changes in linear dimensions for this process –b.

structure, while with further stretching, the structure loses its auxetic properties. In this case, for $\Delta X_1/X_1=0.42$, there is a zero vertical change in dimensions ($X_2/X_2=0$). Phase transition is associated with the indicated critical dimensions.

This tendency occurs for a large group of structures of rotating rectangles (Plewa 2025).

This means that the dimensions in the vertical direction reach the value from the initial state. At the transformation point, there is an asymptote because when $\Delta X_1/X_1 \rightarrow 0.42$, the Poisson's ratio approaches $-\infty$. Such overwhelming auxetic behavior can be achieved through a large range of anisotropic behavior of structures. The significance of this range is that near the occurrence of the asymptote, any arbitrarily large value of the Poisson's ratio can be obtained, both negative and positive. It should be noted that the values $-\infty$ obtained for the Poisson's ratio ν , its inverse $1/\nu$ is zero. This gives the possibility of producing metamaterials with Poisson's ratio equal to zero.

Defining the metamaterial phase transition, one should emphasize once again that in tension, with a continuous change in elongation, there is a sudden transition from the auxetic phase to the non-auxetic phase. This transition can also be obtained in the opposite direction, as during compression with continuous contraction in one direction, there is a sudden change from positive to negative value of the Poisson's ratio.

The presented physical phenomenon of metamaterial phase transition is known from simulation studies, which have effectively anticipated the possibilities of its occurrence.

In the geometric modeling of metamaterial structures, the change of dimensions is a result of movement. It may only be used for specific ranges of dimensional change, which for a given structure is limited by its geometry. Position of the pivot, i.e., the value of the geometric parameter x , must satisfy the condition $x < 1/(2(a/b+1))$ and the maximum value of the angle theta cannot exceed $\arctan(a/b)$ (Plewa 2024). These conditions ought to be applied not only to graphic models but especially to physical structures.

PREVIOUS ACHIEVEMENTS IN THE FIELD OF METAMATERIAL PHASE TRANSITION

Analytical models of solid phase transition confirming non-monotonic stress-strain relationships are being actively developed in the field of computational materials engineering.

This area of research draws inspiration from the theory of phase transition in crystalline solids (Imre 2008, Khajehtourian 2020) and is part of the broader theme of modeling and simulating phase-field transformations in the solid state. Although so far, for mechanical metamaterials exhibiting auxetic properties, the metamaterial phase transition occurs only in simulations, they provide insight into the predictable and programmable, strongly nonlinear movement of the metamaterial (Imre 2008). This way, a relationship is obtained between the critical strain and the phase transition (Liu 2010).

As a result of modeling solid-solid phase transitions in mechanical metamaterials, a phase transition from positive to negative Poisson's ratio was predicted for compression (Wang L. 2022, Hunt 2019, Jiao 2024, Ben-Yelun 2013). It has been shown that for certain geometric parameters of such structures, the Poisson's ratio can vary from positive to negative values (Lim 2024). For this purpose, structures with more than one stable equilibrium configuration were considered, such as (Imre 2008, Wang C. 2023), the flexibility of a two-phase composite with contrasting Young's modulus (Peng 2020) or composites containing different unit cells (Peng 2020) and elastomagnetic metamaterials (Liang X. 2022).

The search for possibilities to confirm such a transition was continued in simulations by inducing phase transitions through various types of stress (Salahshoor 2018), nonlinear deformations (Podesta 2023), elastic waves in a unified network (Chen 2019), and through large deformations (Sorrentino 2021, Kanagae 2023). The theoretical studies considered movements and forces responsible for phase transitions (Bonetti 2017), the phase field model was utilized (Bonetti 2017, Jin 2020, Zawistowski 2024), and an order parameter was introduced, relating the phase transition to the change in the internal order of the metamaterial (Ciarletta

2013). The phase-field method is widely used as an effective computational method for simulating the microstructural evolution taking place during phase transitions in the solid state for metal alloys (Yamaka 2023)

It is known that most phase transitions are abrupt, which is the way in which mechanical properties can change. In the case of mechanical metamaterials, an abrupt change in the value of the Poisson's ratio was expected from $-\infty$ to $+\infty$ (Grima 2008). At the point of such a transition, the Poisson's ratio undergoes a discontinuity.

Theoretical proposals for the implementation of phase transition in mechanical metamaterials involve, among other things, the manufacture of structures made of different unit cells (Peng 2020, Liang Y. 2022) and composites containing various unit cell fillings (Peng 2020).

Despite significant work in the field of design and extensive simulation research, phase transitions of metamaterials have not yet been experimentally validated. The above-mentioned attempts to test the metamaterial phase transition have experienced three main obstacles, i.e., instability and buckling of structures, as well as changes in Young's modulus. That is especially the case since the change in Young's modulus corresponds to the change in material.

One can find an exception that was not classified as a metamaterial transition, i.e., experimental discontinuities in the Poisson's ratio for rotating rhombus structures (Lim 2024).

A different course of these changes was described in another work (Wang L. 2022). The above work deserves particular attention as it examines a 3D structure and, more significantly, at micrometric dimensions. In this work (miniature 3D structure), a continuous transition from negative to positive values of the Poisson's ratio was obtained for some combinations of relative dimensional changes (Wang L. 2022).

Unlike modified structures of rotating rectangles, the change in the value of Poisson's ratio occurs abruptly, which is one of the determinants of the phase transition

Below, we present realizations of rotated rectangle structures for which a metamaterial phase transition

can be found. This was made possible by the applied modification of the rotated rectangle structures and the selection of geometric parameters of the unit cells.

EXPERIMENTAL CONFIRMATION OF METAMATERIAL PHASE TRANSITION

The field of mechanical metamaterial research is dominated by theoretical works featuring interesting analyses conducted by means of simulation. It must be admitted, however, that these works in the virtual realm so far have not contributed to the actual implementation of auxetic metamaterials. Thus, there is a need to demonstrate methods for producing reliably functioning mechanical metamaterials that can change their dimensions without immediate structural failure. One of these proposals includes modified structures of rotating rectangles, for which the effect of metamaterial phase transition has been found. In this case, it concerns a sudden change in the value of the Poisson's ratio, from negative to positive, with a continuous change in the dimensions of the structure.

The basis of the studied structures are rectangular unit cells made of rigid materials. In this particular case, steel sheet and wood-based panels were used. The cut unit cells have holes at the corners, which are spaced away from the edge by a distance equal to $x \times a$ (Figure 1). Such rectangular unit cells are connected by pivots, which take the form of pins, screws, or similar components that provide durable movable connections. The movement of these structures subjected to loading results from the rotation of rectangular unit cells around the pivots. The additional elements in the mechanical nomenclature are called pin-joints and serve as linking and fixing elements. The applied structural system is based on the discrete assembly of a specified set of unit cells and pivots. For practical reasons, elongated rectangular unit cells have been created by combining smaller units. The theoretical relationships of the Poisson's ratio changes with elongation were determined using general analytical relationships (Plewa 2024), and the experimental values were obtained from direct measurements.

The comparison of theoretical and experimental values shown in Figure 3 indicates certain differences. Their source lies in minor inaccuracies in the assembly

process. It is also worth noting that the determined relative values show a large spread due to division by small numbers. The 4×4 structure under consideration shows a very abrupt transition from auxetic to non-auxetic behavior. This transition corresponds to the occurrence of a zero value for the coordinate X_2/X_2 . While the $\Delta X_1/X_1$ coordinate increases linearly, the X_2/X_2 coordinate has a nonlinear trajectory with a maximum value. The respective values at the maximum point of the curve are $\Delta X_1/X_1=0.2385$ and $\Delta X_2/X_2=0.0364$ (Figure 3b).

The location of the phase transformation point shifts to lower strain values for more elongated rectangular unit cells. For higher values of the a/b ratio, the structure loses its auxetic properties at lower tensile deformations.

In Figure 4, the studied experimental structures and their characteristics are presented in the form of the relationship between the Poisson's ratio and the relative expansion. The asymptote on the Poisson's ratio – $\Delta X_1/X_1$ curve lies in this case within lower elongation values, while very large negative Poisson's

ratio values result from small vertical elongation values $\Delta X_2/X_2$.

The two experimental examples not only confirm the occurrence of metamaterial phase transition but also demonstrate the possibility of its fine-tuning. In the phase diagrams (Figures 3 and 4), the Poisson's ratio – degree of deformation shows a particular area corresponding to a sudden transition in auxetic properties, although the symmetry of the system remains unchanged since, for these structures, the auxetic phase has the same symmetry as the non-auxetic phase.

The created modified structures of rotating rectangles serve as tangible evidence of their functionality and the ability to stretch and compress, and in this case, they are used to demonstrate the occurrence of metamaterial phase transition.

Thus, the phase transitions occurring in metamaterials have been experimentally demonstrated. In tension, the structures first increase their dimensions as they are stretched (uniaxially), utilizing the homogeneity of rigid elements and their connections. Such structures

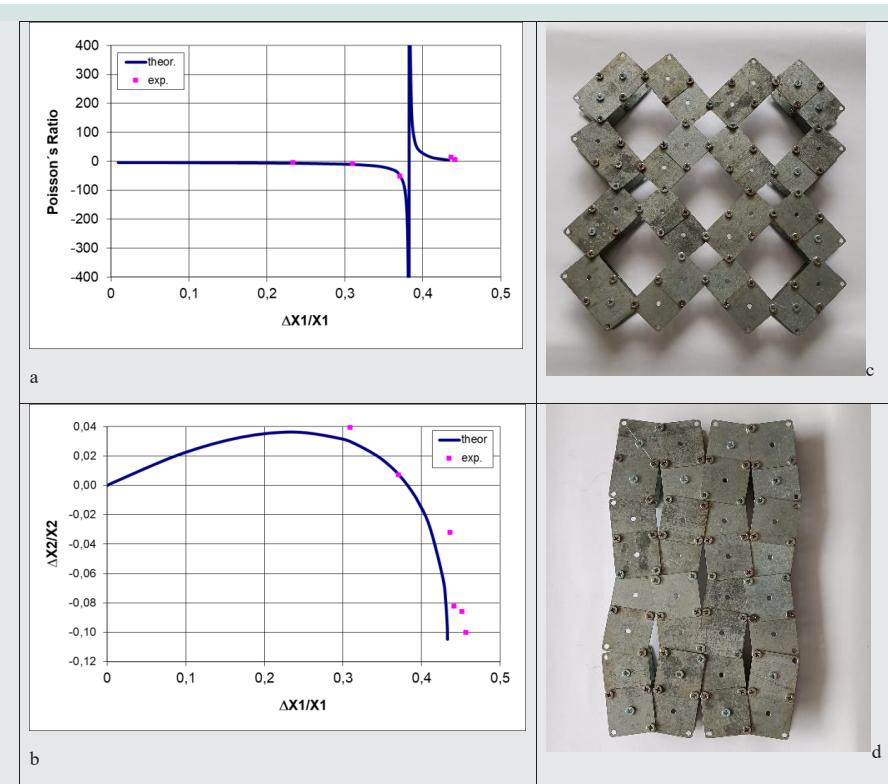


Figure 3: Poisson's ratio as a function of elongation – a, vertical elongation as a function of horizontal elongation – b, and images of 4×4 structure in the *open* (c) position and in the *closed* position (d).

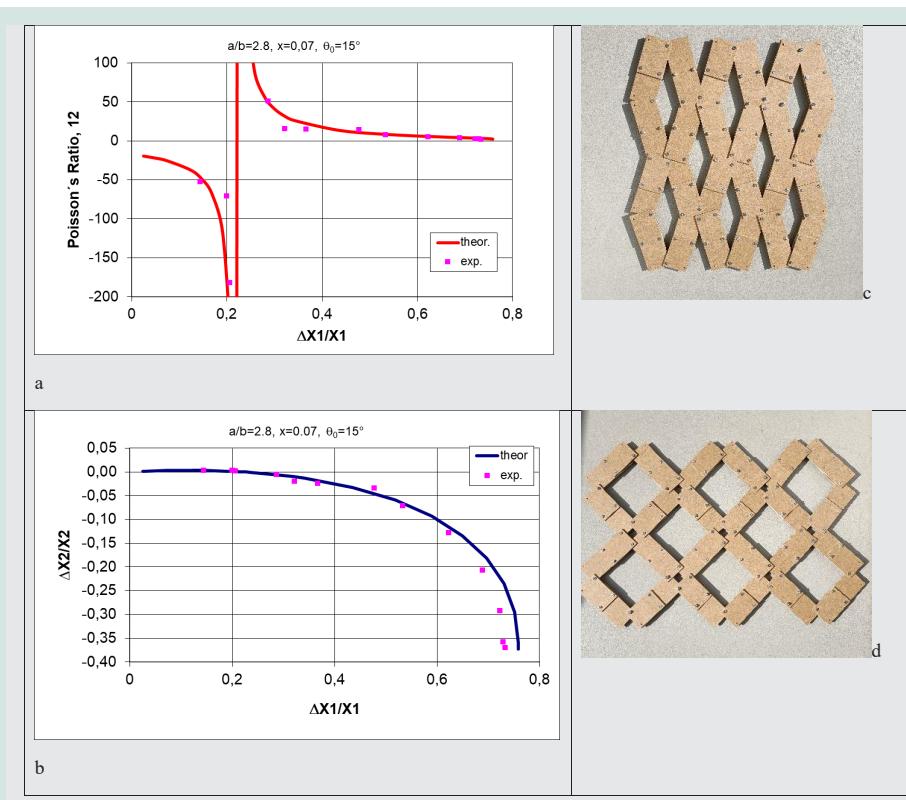


Figure 4: Poisson's ratio as a function of elongation – a, vertical elongation as a function of horizontal elongation – b, and image of the 6X4 structure in the *closed* (c) and *open* (d) position.

are practically reliable for any number of rectangular unit cells. Then, when further stretched, the structures slightly contract, which makes the change in dimensions go from negative to positive. The relative change in dimensions depends on the direction of stretching, which is also expressed by the values of the Poisson's ratio v and $1/v$.

CONCLUSIONS AND DISCUSSION

The various approaches to metamaterial phase transition analysis outlined above are examples of valued theoretical creativity. The analyses, comparisons, and generalizations presented there became an inspiration for identifying an actual physical metamaterial phase transition. The phase transition presented in this work, involving modified rotating rectangular structures, exhibits certain particular properties, especially differences regarding the assumptions made in the simulations. First of all, there are no phase boundaries, in this case, between the auxetic phase and the non-auxetic phase. In this case, the given structure first exhibits auxetic behavior, followed by non-auxetic behavior. This differs from the established theory of sharp phase boundaries, as well as

the two phases being in equilibrium. In other words, it refers to a single metamaterial with a constant structure that first exhibits negative and then positive values of the Poisson's ratio. The presented structure is capable of undergoing a phase transition from a positive to a negative Poisson's ratio.

In the studied system, there is an effective transmission of an external force causing a continuous change in dimensions, that is, a constant monotonic stretching proceeding through successive stable positions of the unit cells in the structure. This dynamic behavior of the metamaterial involves constant deformation and lacks equilibrium states. After the auxetic-non-auxetic phase transition takes place, the progressive change in dimensions continues. In the case of stretching, the limit is the value of the theta angle, which cannot exceed the value of $\arctan(a/b)$ (Plewa 2024).

The special feature of the presented metamaterial phase transition for modified rotating rectangle structures is its abrupt course and the attainment of very large negative and positive values of Poisson's ratio. The course of Poisson's ratio–elongation curves is discontinuous. This phase transition is analogous to

first-order phase transitions.

In comparison, the phase transition found for spatial lattice structures is not (Wang L. 2022) abrupt, and the characteristic curve has a continuous course. In this case, there is a discernible similarity to a second-order phase transition. The explanation for the differences in the nature of both types of phase transitions relates to the mechanism of dimensional changes. Indeed, for the structure of the modified rotating rectangles, it occurs due to pure hinging (rotations of unit cells around the pivots). However, in the case of a spatial lattice structure, this change is due to the bending of the flexible parts of the structure (Wang L. 2022). The squeezed 3D microstructure shrinks in such a way that, in some directions, it initially shows auxetic properties, and then, with further shrinkage, it exhibits non-auxetic properties. This 3D mechanical metamaterial has been shown to be capable of a phase transition from positive to negative Poisson's ratio under compression. Poisson's ratio in both of the discussed structures is not constant and varies with deformation and the initial geometric parameters of the structures.

The common feature of these two different metamaterial phase transitions is that there is no equilibrium of the two phases at the transition point. Structurally, it is the same phase whose properties change with the changing conditions. Although the phase transition separates states of the structure with different characteristic properties, it is still a structure with the same symmetry. The same structure can exhibit both positive and negative Poisson's ratio (Grima 2004).

The relevant literature offers some insights as to the practical usefulness of such phase transitions. It is expected that phase transitions in metamaterials will improve performance capabilities in energy management (Liang X. 2022), and through polymorphic reconfiguration, they will even allow for self-repair of structures (Hwang 2022). In solid-state physics, phase transitions can affect the functionality of materials and change their properties. Phase transitions of metamaterials yield the promise of propulsive movement and management of high-speed energy transfer events (Liang X. 2022).

In summary, it can be emphasized that this work presents modified structures of rotating rectangles that exhibit significant dimensional changes without cracking. By using additional elements in the form of pivots, much greater elongation values are achieved than those found in unmodified solutions. This allows a mechanical response to external forces that leads to very high values of the Poisson's ratio in the phase transition area. By adjusting the geometric parameters of unit cells, one can control the behavior of the structure under deformation and achieve a tunable change in the sign of Poisson's ratio. The physical response to a continuous change in deformation can either be monotonic, i.e., corresponding to a negative value of the Poisson's ratio, or non-monotonic when the relative change in elongation reaches a zero value, and the structure undergoes a metamaterial phase transition from auxetic to non-auxetic.

The contribution of the present work is that it first analytically and then experimentally demonstrates the occurrence of this transition using a real, tangible structure. The realistic mechanical response of structures to loading and the experimentally observed metamaterial phase transition can be considered progress in this area.

ACKNOWLEDGMENT

Among artificial materials, there is a group of mechanical metamaterials that exhibit unusual properties under loading. In tension, these materials expand in length and width and contract in compression. Such metamaterial behavior is called auxetic, and it is distinguished by a negative Poisson's ratio. For these metamaterials, the occurrence of a phase transition was predicted but has not been confirmed experimentally so far. By stretching structures of rotating rectangles, as the elongation undergoes continuous change, there is a rapid change in the Poisson's ratio from negative to positive values. The opposite effect can be obtained by compressing the stretched structure. This phenomenon can be classified as a solid phase transition.

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DATA AVAILABILITY STATEMENT

The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding author.

CONFLICTS OF INTEREST

The author declare no conflicts of interest. The funders had no role in the design of the study in the collection, analyses, or interpretation of data; in the writing of the manuscript; or in the decision to publish the results.

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