

10<sup>th</sup> International Conference

**Auxetics and other materials and models  
with "negative" characteristics**

15<sup>th</sup> International Workshop

**Auxetics and related systems**

2<sup>nd</sup>–6<sup>th</sup> September 2019  
Będlewo, Poland



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## A few historical remarks

The history of scientific meetings focused on auxetics (materials that expand/ contract their transverse directions while under lateral stretch/compression) and other unusual materials, reaches back to the years 2004 and 2005, when the first two international workshops were organised in Będlewo near Poznań (Poland). Both meetings took place in the Mathematical and Research Conference Center (MRCC). So far the tradition of annual meetings of scientists and engineers working in the field of auxetics and other systems of “negative” characteristics has been continued (with sole exception in the year 2013) to this day. Besides Będlewo (Poland) in 2004 and 2005, auxetic meetings have been organised in Exeter (United Kingdom) in 2006, Msida (Malta) in 2007, Bristol (United Kingdom) in 2008, Bolton (United Kingdom) in 2009, Gozo (Malta) in 2010, Szczecin (Poland) in 2011, Bolton (United Kingdom) in 2012, Poznań (Poland) in 2014, Msida (Malta) in 2015, Szymbark near Gdansk (Poland) in 2016, Heraklion (Crete, Greece) in 2017, and Sheffield (United Kingdom) in 2018.

The meetings have brought together **three groups that seek to explain** the origins of unusual elastic properties of materials, groups that model structures exhibiting auxetic properties, as well as groups that aim at real life applications of materials with auxetic properties. Each meeting serves as a platform on which the theory meets applications. Traditionally, after each conference, selected contributions are published, after a rigorous peer review. The first volume with papers related to the Auxetic Meetings was published in the special issue of Computational Methods in Science and Technology (CMST), which is published by the Poznań Branch of the Polish Academy of Sciences (PAS) and Poznań Supercomputing and Networking Center affiliated at the Institute of Bioorganic Chemistry of the PAS, see: [http://cmst.eu/issue/issue.2004\\_volume.10\\_2/](http://cmst.eu/issue/issue.2004_volume.10_2/). The next ‘auxetic’ volumes were published as special/thematic issues of Physica Status Solidi B (PSSb) published by Wiley, see: <https://onlinelibrary.wiley.com/journal/15213951>. Thirteen such issues were published to date with the Guest Editors as follows:

- Krzysztof W. Wojciechowski, Andrew Alderson, Arkadiusz Brańka, Kim L. Alderson, Preface, vol. **242(3)**, 497 (2005).
- Krzysztof W. Wojciechowski, Andrew Alderson, Kim L. Alderson, Bogdan Maruszewski, Fabrizio Scarpa, Preface, vol. **244(3)**, 813 – 816 (2007).
- Christopher W. Smith, Krzysztof W. Wojciechowski, Preface, vol. **245(3)**, 486 – 488 (2008).
- Joseph N. Grima, Krzysztof W. Wojciechowski, Preface, vol. **245(11)**, 2369 – 2372 (2008).
- Chrystel Remillat, Fabrizio Scarpa, Krzysztof W. Wojciechowski, Preface: Auxetics and Other Unusual Systems, vol. **246(9)**, 2007 – 2009 (2009).
- Kim L. Alderson, Andrew Alderson, Krzysztof W. Wojciechowski, Preface: Auxetic Materials and Related Systems, vol. **248(1)**, 28 – 29 (2011).
- Ruben Gatt, Joseph N. Grima, Jakub W. Narojczyk, Krzysztof W. Wojciechowski, Preface: Auxetic Materials and Related Systems, vol. **249(7)**, 1313 – 1314 (2012).

- Krzysztof W. Wojciechowski, Joseph N. Grima, Kim L. Alderson, Jarosław Rybicki, Preface: Auxetic Materials and Related Systems, vol. **250(10)**, 1959 – 1962 (2013).
- Kim L. Alderson, Andrew Alderson, Joseph N. Grima, Krzysztof W. Wojciechowski, Preface: Auxetic Materials and Related Systems, vol. **251(2)**, 263 – 266 (2014).
- Krzysztof W. Wojciechowski, Fabrizio Scarpa, Joseph N. Grima, Andrew Alderson, Preface: Auxetics and other systems of “negative” characteristics, vol. **252(7)**, 1421 – 1425 (2015).
- Krzysztof W. Wojciechowski, Fabrizio Scarpa, Joseph N. Grima, Andrew Alderson, Preface: Auxetics and other systems of “negative” characteristics, vol. **253(7)**, 1241 – 1242 (2016).
- Krzysztof W. Wojciechowski, Fabrizio Scarpa, Joseph N. Grima, Andrew Alderson, Preface: Auxetics and Other Systems of Anomalous Characteristics, vol. **254(12)**, 1770266 (2017).
- Krzysztof W. Wojciechowski, Fabrizio Scarpa, Joseph N. Grima, Andrew Alderson, Preface: Auxetics and Other Systems of Anomalous Characteristics, vol. **256(1)**, 1800736 (2019).

The covers of the thematic issues related to the Auxetic Meetings can be seen in Fig. 1 and the following individuals co-authored the articles selected by the PSSb Staff Editors as the front cover or back cover papers: Wm. G. Hoover, C. G. Hoover (2005); S. Xinchun, R. S. Lakes (2007); V. R. Simkins, N. Ravirala, P. J. Davies, A. Alderson, K. L. Alderson (2008/03); L. Dong, D. S. Stone, R. S. Lakes, Q. Liu, J. Yang, X. Sun, X. Cheng (2018/11); P. Pikhitsa, M. Choi, H.-J. Kim, S.-H. Ahn, C. Lira, F. Scarpa, M. Olszewska, M. Celuch (back cover) (2009); S. A. McDonald, G. Dedreuil-Monet, Y. T. Yao, A. Alderson, P. J. Withers (2011); D. M. Kochmann (2012); Y.-C. Wang, C.-C. Ko (2013); R. Gatt, R. Caruana-Gauci, D. Attard, A. R. Casha, W. Wolak, K. Dudek, L. Mizzi, J. N. Grima (front cover), J. Lisiecki, S. Kłysz, T. Błażejewicz, G. Gmurczyk, P. Reymer (back cover) (2014); S. Czarnecki, P. Wawruch (front cover), A. Airolidi, P. Bettini, P. Panichelli, M. F. Oktem, G. Sala (back cover) (2015); L. Zhou, L. Jiang, H. Hu (front cover), T.-C. Lim (back cover) (2016); J. N. Grima-Cornish, J. N. Grima, K. E. Evans (front cover), Y.-C. Wang, M.-W. Shen, Si-M. Liao (back cover) (2017); D. T. Ho, C. T. Nguyen, S.-Y. Kwon, S. Y. Kim (front cover), J. W. Narojczyk, K. W. Wojciechowski, K. V. Tretiakov, J. Smardzewski, F. Scarpa, P. M. Piękowski, M. Kowalik, A. R. Imre, M. Bilski (back cover) (2019).

In this year, 2019, the Jubilee Meeting (the 15th International Workshop and 10th International Conference) has returned to Bedlewo and is organised by the Institute of Molecular Physics (IMP) of the PAS. For this reason we very briefly mention the history of Bedlewo and the history of the IMP PAS below. The remarks below and photographs are based on materials obtained from Mr. Sławomir Malecha, the administrative manager of the MRCC, and from the administration of the IMP PAS.





Figure 1: Covers of the special/thematic issues related to auxetic meetings.

*The Mathematical Research and Conference Center* is located in the village Będlewo, about 30 km southwest from Poznań. The earliest mentions of Będlewo in the history of Poland reach back to the end of XII century, when the area was ruled by Będlewczy family. Since XVII century Będlewo was ruled by the



Greater Poland branch of the Potocki family. One of the more noteworthy rulers of Będlewo was Bolesław Potocki (1861-1898) who enlarged the land properties. After his 37 year rule they included Będlewo, Wronczyn, Dymaczewo, Zamysławo, Srocko, Wojnowice, Dakowe Mokre, in the total area of 4,728 ha. He was also the founder of KLIWECKI, POTOCKI and SKA Bank, a member of the Theatrical Committee, and he dedicated the land to the Polish Theatre. In 1866 the Palace in Będlewo was renovated. The manor house with thatched roof was built. In 1939 Będlewo was ruled by Elizabeth from Międzyńscy Ledóchowscy family. During the Second World War Germans destroyed all the portraits of Polish kings and all the decorations. After the Second World

War the palace underwent a number of reconstructions. In 1976 the Poznań Branch of the Polish Academy of Sciences obtained the palace and turned it into the Creative Work Centre. In 1996 the Palace has been overturned to the Mathematical Institute of the Polish Academy of Sciences. The Conference Centre was established and then quickly developed. In 1997 a new building that now houses the hotel has been built, the lecture room, the farm entrance (the building with the reception and a tower with the bell), courtly outhouse, and the stable had followed. The lakes and the ponds were renovated. Presently the Palace functions as a Mathematical Research and Conference Centre of the Polish Academy of Sciences. The Centre can accommodate 150 people during a lecture. Many





well-known mathematicians, artists, politicians and contractors visited Będlewo palace.

Today, when entering the palace one can see a beautiful hall with an authentic floor, wooden banister with Potocki armorial bearings. To the left the Knight chamber (the biggest one) is located. Inside the chamber, on the walls one can see the grey polychromes with Potocki and Pilawa armorial bearing. From there one enters a hall which used to be a library. It has a beautiful wooden fireplace, reconstructed fabric wallpaper, wood panelling and stuccos on the ceiling. To the right, there is a chamber in the rococo style where one can also see reconstructed fabric wallpapers and stuccos on the ceiling. Next one enters the round room with the reconstructed claret niches and the copies of antique statues. There are also fireplaces made of white marble. Up the stairs, on the first floor there are rooms that served the family and guests. All rooms on the ground and first floor were decorated in the neo-Gothic style. At present these rooms are not used. The palace is surrounded by a park which covers about 9 ha. The park is in an English style which joins the elements of the forest. Some unique trees (under the protection of the law) can be found here. In front of the palace a marble fountain can be seen, and in the back, two ponds and the terrace full of flowers can be found.







The history of the *Institute of Molecular Physics Polish Academy of Sciences* in Poznań goes back to 1953, when the Institute of Physics of the Polish Academy of Sciences in Warsaw established a branch in Poznań - the Ferromagnetics and Ferroelectrics Department led by Professor Dr. habil. Szczepan Szczeniowski. In 1956 a new, Dielectrics Department was established under the direction of Professor Dr. habil. Arkadiusz Piekara. The next milestone came in 1966, with the establishment of the Radiospectroscopy Department led by Professor Dr. habil. Jan Stankowski. Finally, the Institute of Molecular Physics of the Polish Academy of Sciences in Poznań at its current form was proclaimed in 1975, as an autonomous institute of the Polish Academy of Sciences. Its first director was Prof. Dr. habil. Jan Stankowski and the Chairman of the Scientific Council was Prof. Dr. habil. Jerzy Małecki. Since 2018, Prof. Dr. habil. Zbigniew Trybuła holds the position of the director and the Chairman of the Scientific Council is Prof. Dr. habil. Roman Micnas.

The IMP PAS is organized into 14 departments grouped into 3 divisions, which are led by Prof. Dr. habil. Jadwiga Tritt-Goc, Dr. habil. prof. IMP PAS Tomasz Toliński, and Prof. Dr. habil. Krzysztof Witold Wojciechowski, respectively. Over 110 employees work at the Institute and about 20 doctoral students. It includes 12 Professors, 14 associate professors, 31 doctors, 21 engineers, one librarian, as well as administrative and technical support employees. The Institute's research work mainly involves fundamental investigations in condensed matter physics, with 14 research laboratories applying both experimental and theoretical methods. IMP PAS is the only Institute of the Academy, which has a scientific department - Department of Low Temperature Physics - located directly in the area of a manufacturing plant of Polish Oil and Gas Company. Each year the Institute's staff members publish circa 100 articles in international journals and present approximately 180 papers at national and international conferences. Roughly half of those are developed in cooperation with foreign partners. The Institute's Scientific Council, which includes its own independent research employees as well as eminent scientists from various Polish research centres, possesses the right to confer doctorate (PhD) and doctor of science (DSc) degrees. The IMP PAS groups are experienced in advanced studies on low dimensional as well as bulk systems and the laboratories are equipped in modern apparatus for samples preparation

and characterization. Research realized in IMP PAS concerns mainly condensed matter physics with a special focus on:

- theoretical and experimental physics of magnetics (thin films, amorphous magnetics, electronic structure);
- physics of ferroics (ferroelectrics, superprotonic conductors, electrets, piezopolymers);
- liquid crystals (ferroelectric and antiferroelectric materials);
- crystalline molecular conductors and fullerenes;
- spintronics, meso- and nanoscopic systems;
- superconductivity and low-temperature physics;
- electron paramagnetic resonance (EPR);
- magnetic resonance micro-imaging (MRI);
- computer simulations of colloids;
- computer simulations and theoretical studies of auxetics and related metamaterials.

The Institute is a member of various scientific organizations and its researchers participate in diverse scientific projects. For instance, the Institute is the leader in the project the National Centre for Research and Development - PIHe3, which focuses on obtaining the  $^3\text{He}$  isotope from a liquid helium. One of the goals of the Institute is to educate and guide early-stage researchers. Every year a number of students from Adam Mickiewicz University (UAM) in Poznan and Poznan University of Technology (PUT) write their dissertations under the patronage of the Institute's researchers. Because of the close cooperation existing between the IMP PAS, UAM and PUT outstanding students can continue their research at the International Doctoral Studies. In addition, the NanoBioMedical Centre of UAM and the IMP PAS are co-leaders of the Interdisciplinary Doctoral Studies in Nanotechnology-Electronics and Photovoltaics funded by the European Union (POKL.04.03.00-00-015/12). As a part of this program, doctoral students are required to complete a six-month internship abroad. The IMP PAS puts also a great emphasis on a promotion of science in society, especially secondary and high school students. Annually, since 1985, the Department of the Low Temperature Physics organizes workshops called 'Summer with Helium' addressed to high school students interested in physics. For a one week the participants are allowed to conduct research and their results are presented during final seminar. Since 2009, researchers from the Department of the Low Temperature Physics have led an extracurricular science club for secondary school pupils. After each year, the results are presented in a form of interactive exhibition, which is seen by about thousand visitors. The Institute's researchers participate in, and coordinate, numerous international and local conferences. The one with the longest tradition is now-called "The European Conference Physics of Magnetism" (PM). The Conference has been co-organized, every three years since 1975, with the Faculty of Physics UAM. Other conferences worth to be mentioned are: Polish-Czech Seminar on Structural and Ferroelectric Phase Transition, and Auxetics and Related Systems.



# ABSTRACTS





# Response and energy absorption capabilities of chiral topologies in plastic range

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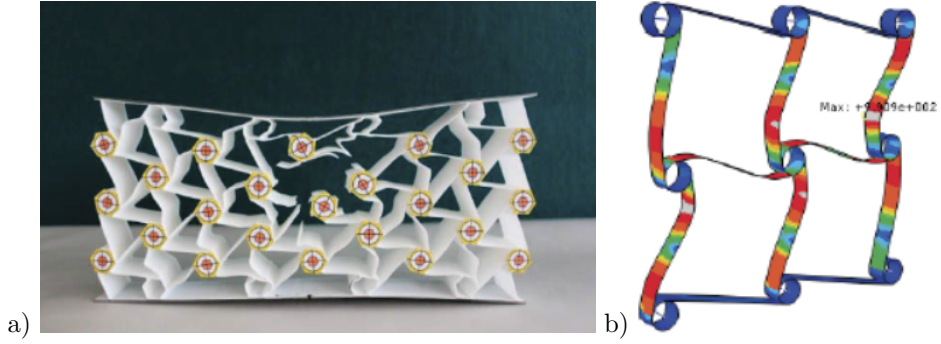
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The results of many studies have confirmed the possibility to develop chiral cellular structures with auxetic behaviour in elastic range [1]. Nevertheless, many important applications suggested for auxetic cellular structures are related to energy absorption and relies on the response of these structural topologies in the inelastic field [2,3]. Experiments carried out by using 3D-printed polymeric chiral absorbers indicated that the exploitation of the energy absorption potential of such cellular structure depends on the auxetic response in the plastic range and on the reduction of ligament failure events during the deformation process (Fig. 1-a).

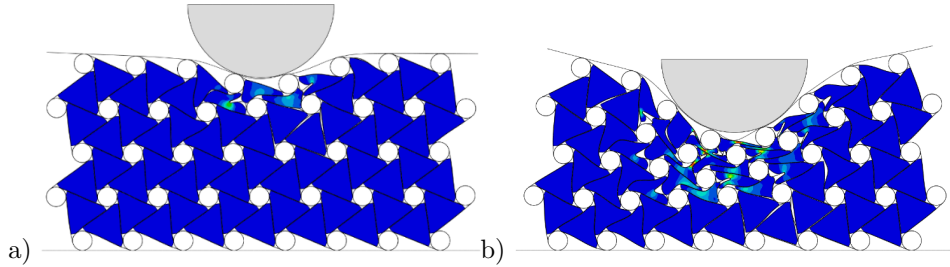
Therefore, numerical studies have been conducted to maximize the auxetic response in plastic range of exachiral and tetrachiral cells. Parametric finite element models with tapered ligaments have been automatically generated by varying all the geometrical characteristics (Fig. 1-b). Analyses have been conducted to evaluate the transversal contraction of compressed cells before ligament failure, which has been predicted by monitoring the maximum plastic strains in the elements. Sensitivity studies have been performed to establish the scaling law for the forces generated during the compression and for the maximum contraction achievable before failure. The use of a genetic algorithm made possible the identification of the most promising geometries to maximize the contraction of the cellular structures.

Such geometries have been used to generate possible configurations for chiral honeycombs filled by polymeric foam, which have been simulated by using a numerical approach validated in a previous experimental campaign, which also include the prediction of ligament failure to improve the reliability of predictions.

Results indicate that the combination of chiral structure and foam, and the use of geometries delaying ligament failure, may represent important ingredients to develop innovative and efficient absorbing devices. Indeed, the geometries identified in the optimization process have exhibited very high energy absorption capabilities in the case of localized impacts, compared with the ones obtained by the chiral structure and by the foam separately considered.



**Figure 1.** Experiments on a polymeric exachiral absorber a) and model to maximize auxetic response in plastic range b).



**Figure 2.** Numerical simulation of foam-filled auxetic honeycomb in impact conditions.

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# Smartly designed composite structures with tunable thermomechanical properties

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Most materials exhibit positive Poisson's ratio (i.e. get thinner when stretched), compressibility (i.e. shrink when subjected to a compressive hydrostatic pressure) and thermal expansion (i.e. expand when heated). However, it is not uncommon for some materials or structures to exhibit negative values for these properties. This work presents conceptual composite cellular structures with tunable thermomechanical properties. These structures are wholly made out of materials that exhibit conventional thermal and mechanical properties but are designed in such a way that, through modification of parameters defining these systems, their overall thermomechanical properties can be modified and tailored to exhibit negative values.

# Discrete modelling and simulation of auxetic lattice materials

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Artificial periodic cellular (lattice) materials attract the attention of researchers due to their outstanding stiffness and strength and enhanced absorption of mechanical energy at relatively small density. Lattice materials can be relatively easily fabricated using modern additive technologies. Computer simulations can help to choose the best cell topology, a number of cells, geometry of struts, material properties. Usually FEM is used for simulations, however, in some cases, discrete models seem to be more applicable. For instance, such problems include big deformations, buckling, and fracture of cellular materials.

In this work, two discrete models are proposed to describe linear deformation in auxetic lattices. Two-parametric model is used for qualitative analysis of cellular auxetic and conventional materials. The model describes an interaction between the cells' nodes with axial and torsional linear springs. The homogenization procedure is proposed to determine the effective properties of solid material corresponding to the re-entrant and regular honeycombs. The procedure is based on a comparison of strain energies of the structures and corresponding orthotropic material. The components of the stiffness tensor and Poisson's ratio of the structures are obtained as a function of interaction parameters and the angles between the structural elements.

Although the two-parametric model can accurately describe the properties of the isotropic 2D material, it lacks the accuracy in the anisotropic case. Due to this, more complicated models based on the interaction of the particles with the rotational degrees of freedom are used for more realistic simulations. One of them is a linear elastic model, another one is the enhanced vector-based model or EVM [1]. For the linear model, also an analytical procedure of homogenization is proposed. Both models consider lattice material as a set of particles connected by the potential of interaction. The parameters of the potential are related to linear elastic longitudinal, transverse (shear), bending, and torsional stiffness. As a result, every strut of cellular material is modeled with two particles with an elastic bonding. Examples of the simulation of the fracture and wave-propagation in lattice materials are proposed. It is shown, that the results are in good correspondence with the experimental and finite element results obtained by the other authors.

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# Equation of state and phase diagram of soft cyclic hexamer systems in two dimensions

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Monte Carlo simulations of two-dimensional systems of particles interacting via a nearest-neighbour  $n$ -inverse-power site-site potential [1], further referred to as soft cyclic hexamers (SCH), were performed. The single SCH molecule consists of a hard regular hexagon of the side  $\sigma$  (the core of the particle) and six *soft* discs, which are centred at the vertices of the hexagon. The discs are characterized by an “atomic parameter”  $d$ , which can be thought of as their diameter. The dimensionless ratio  $d^* = d/\sigma$  can be used to define the molecular anisotropy of the hexamers,  $\alpha = 1/d^*$ . The  $n$ -inverse-power intermolecular potential is defined as:

$$u(r_{ij}, \phi_i, \phi_j) = \sum_{\alpha, \beta=1}^6 \left( \frac{d}{r_{ij}^{\alpha\beta}} \right)^n, \quad (1)$$

where  $r_{ij}^{\alpha\beta}$  is the distance from the site  $\alpha$  of molecule  $i$  to the site  $\beta$  of molecule  $j$  and  $\phi_i$  represents the orientation of molecule  $i$ . In addition to this, the hard cores of molecules also interact, so the configurations with overlapping hexagons are forbidden - their energy is infinite. Systems of hard cyclic hexamers (HCH) were studied previously [2,3] and they have been shown to form elastically isotropic phases, the densest of which is chiral and exhibits negative Poisson’s ratio [1,4,5]. Such materials are presently known as auxetics [6–8] and they exhibit very interesting anomalous elastic properties [9,10]. In the present work computer simulations were used to determine the equation of state and phase diagram of analogous SCH molecules for  $d^* \in [0.5, \infty)$ . Furthermore, a comparison of the studied characteristics of SCH with the HCH model was made.

## Acknowledgements

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# On the auxetic properties of anisotropic 2D crystalline media

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Progress in developing different low-dimensional structures like thin solid films, different types of monolayers and quasi-2D structures requires useful approaches for determining their elastic properties, in particular their auxetic behavior. As such structures may be well described as 2D media the development of simple and effective analysis of auxetic behavior of 2D model material of different symmetries is of considerable interest and needs further development.

In the presentation, a description of the auxetic behavior of quadratic 2D materials under hydrostatic pressure based on the X,Y-ratios of the elastic moduli will be presented. It will be shown that the XY-plane approach developed for cubic 3D materials can be exploited to describe the auxetic behaviour of quadratic or 2D cubic materials which is the highest nonisotropic 2D crystal symmetry.

Within the proposed framework one can search for microscopic interactions which place the material in the target nonauxetic, auxetic, or partially auxetic region in the XY-plane. As a step in such an investigation we considered 2D simple static model systems of particles interacting via the pairwise spherically symmetric potential. With the selected model solids it will be demonstrated how the different main parts of the interaction influence the 'position' in the XY-plane. In particular it will be shown that the tethered particle system can exhibit different auxetic behaviour through a simple compression-tension mechanism.

The corresponding approach for the rectangular symmetry 2D materials will be discussed. Some differences in auxetic behavior of the quadratic and rectangular symmetry 2D materials will be mentioned.

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# Behaviour of topology optimized auxetic structures under static loading

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The auxetic structures have unique properties that differ them from solid structures - it is negative Poisson ratio. The most common auxetic metamaterials are arranged in foams or cellular structures. One of their key property is low density and ability to dissipate energy. Such structures were successfully manufactured from polyurethane [1].

In first part, authors present four structures (re-entrant, tetrachiral, lozenge grid and 4-STAR grid). This structures are then used in topology optimisation process [2]. The aim of this operation was to maintain stiffness of the structure with mass reduction. The remaining mass was between 10% and 90%, with step of 5%. Based in this results, three-dimensional CAD models were developed.

In the second part of this paper, authors conducted finite element analysis to determine resulting stiffness of optimised structures under static loads and prescribed displacements. Material properties, boundary conditions and loads were similar in all cases. Highly elastic material with low stiffness was used in simulations, by the name of thermoplastic polyurethane (TPU). In final section, results were presented and discussed. The optimal mass of structure was determined by comparing total displacement of structures with the same load.

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# Recovery of the underlying microstructures appearing in two- and three-dimensional least compliant elastic bodies

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The problem of recovery of the microstructure of the least compliant bodies made of inhomogeneous isotropic material will be presented. The Isotropic Material Design (IMD) delivers the optimal distribution of the bulk  $k$  and shear  $\mu$  moduli within the design domain ensuring the highest stiffness of the two- and three-dimensional (i.e. 2D and 3D) linearly elastic bodies [1,2].

In two-dimensional case, the varying underlying microstructures, i.e. the Representative Volume Elements (RVE) constructed of one or two isotropic materials corresponding to the optimal designs constructed by IMD method is recovered by matching the values of the optimal  $k^*$ ,  $\mu^*$  moduli with the values of the effective moduli  $k^H$ ,  $\mu^H$  of the RVE computed by the theory of homogenization.

The three-dimensional microstructure is constructed by a subsequent laminations of the two isotropic materials of ordered properties repeated six times in the directions  $\mathbf{n}_1$ ,  $\mathbf{n}_2$ , ...,  $\mathbf{n}_6$  of the vertices of the icosahedron. The composite is constructed by the subsequent laminations: 1) of the strips of the isotropic material of moduli  $k_1$ ,  $\mu_1$  (defining isotropic tensor  $\mathbf{C}^1$ ) and of moduli  $k_2$ ,  $\mu_2$  (defining isotropic tensor  $\mathbf{C}^2$ ) such that  $k_1 < k_2$  and  $\mu_1 < \mu_2$ , which is called the ordered case; this leads to the material called “ $h_1$ ”, 2) of the strips of the stronger material of moduli  $k_2$ ,  $\mu_2$  with the material “ $h_1$ ”, which leads to the material “ $h_2$ ”, ..., 6) of the strips of the stronger material of moduli  $k_2$ ,  $\mu_2$  with the material “ $h_5$ ”, which leads to the 6th rank isotropic laminated composite “ $h = h_6$ ” defined by Hooke tensor  $\mathbf{C}^h$  [3].

Each microstructure is characterized by a finite set of parameters and the main task is to find them. This task requires special analytical and numerical tools. The resulting bulk and shear moduli are equal to the upper Hashin and Shtrikman bounds. It was shown numerically that by combining a weak (compliant) isotropic material (defined by  $k_1$ ,  $\mu_1$  moduli) with a strong (stiff) isotropic material (defined by  $k_2$ ,  $\mu_2$  moduli) it is possible to design an isotropic composite closest to the optimal one found by IMD method.

In both: 2D and 3D case, the ability to model an auxetic behavior within the subdomains where the optimal Poisson’s ratio assumes negative values is also shown.

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# Impact resistance of mechanical metamaterials with magnetic and nonmagnetic inclusions

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In this work [1], through the use of molecular dynamics simulations, we analyse the behaviour of a particular mechanical metamaterial with different types of magnetic and nonmagnetic inclusions. In particular, we investigate the potential of such systems to withstand a collision with an external body. As a result of our studies, we show that the use of appropriately distributed magnetic inclusions may significantly enhance impact resistance of the system in comparison to its nonmagnetic counterpart. In addition to that, it is shown that the extent of the exhibited impact resistance strongly depends on the orientation and distribution of magnetic inclusions within the structure. This means that protective properties of the system may be solely controlled via the way how magnetic inclusions are inserted into the structure. It should be also emphasised that the results discussed in this work may be used in order to enhance impact resistance of already existing protective devices that attribute their properties to the structural design and elastic properties of constituent elements.

## Acknowledgements

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# Magnetic properties of dense systems of magnetic nanoparticles prepared in non-magnetic auxetic matrices

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Dense assemblies of magnetic nanoparticles in non-magnetic auxetic matrices belong to a class of magneto-auxetic systems [1]. Their magnetic properties can be controlled both via an axial deformation of the matrix which process affects the interaction between magnetic nanoparticles and by an external magnetic field. The consequence of the magneto-elastic coupling in these metamaterials can be the observation of a large cooling/heating effect without the presence of the external magnetic field even at room temperature [2]. The use of the external magnetic field is an additional mechanism allowing to increase the extent of the magnetocaloric effect. In this presentation, examples will be shown of how the auxeticity of magneto-mechanical materials can be used to control their magnetocaloric properties.

## Acknowledgements

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# Magnetic inclusions in non-magnetic auxetic matrices

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The presentation concerns a class of metamaterials which are magneto-auxetics [1]. To prepare such metamaterials one can use magnetic components embedded into the non-magnetic auxetic matrix. Often, magneto-auxetic models are represented by a bead-spring model as in the early publication focused on modelling of the auxetic ferrogel [2]. In this type of metamaterials the magnetic ordering strongly depends on elastic deformation of the non-magnetic matrix and the value of the external magnetic field.

Magnetic inclusions inserted into an otherwise nonmagnetic structure can be utilised in a number of ways with one of the more interesting examples being the possibility of inducing the magnetocaloric effect [3]. As discussed in the literature, magnetocaloric properties of such materials can be induced upon applying a mechanical strain to the structure even at zero external magnetic field. In this presentation we show how the mechanical deformation of the non-auxetic matrix affects the magnetic ordering and, consequently, magnetocaloric properties. We also refer to the publication [4] in which it was shown how the rate of deformation can affect magnetic ordering and hence control the magnetic properties of the whole system.

## Acknowledgements

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# Auxetic closed cell foam by steam processing, a parametric study

O. Duncan<sup>1,2</sup>, T. Allen<sup>2</sup>, L. Foster<sup>3</sup> and A. Alderson<sup>1</sup>

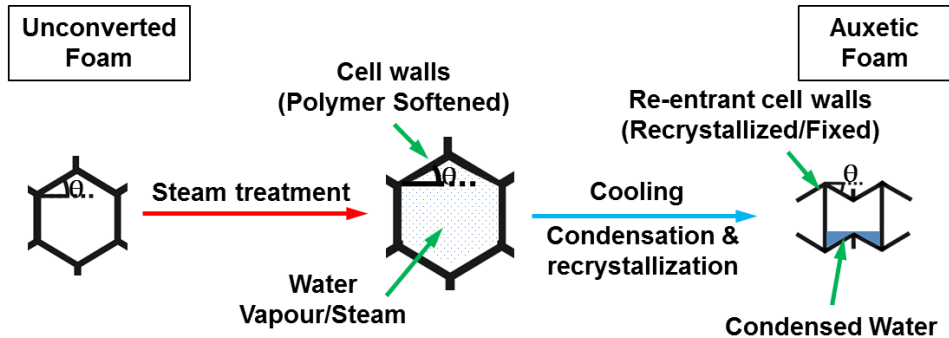
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Increasing concern over the limitations of protective equipment has prompted development calls from sports participants, teams and governing bodies, and defence institutions such as the UK's Defence, Science and Technology Laboratory. Auxetic materials, with high energy absorbance, indentation resistance and conformability have been regularly discussed as a potential solution. One of the difficulties in applying auxetic foams to protective equipment is that their Young's modulus is substantially lower (approximately 30 to 100 kPa [1]) than closed cell foam often used in personal protective equipment ( $\sim 1\text{MPa}$  [2]).

To date, only limited reports of auxetic closed cell foam conversions have been reported, with the methods typically using pressure vessels [3]. A recent method [4] uses steam absorption followed by condensation, causing cell contraction (Figure 1). The simple method could create a step change in auxetic closed cell foam fabrications. A parametric study into the effect of the duration of steam treatment on cell shape (obtained via micro-ct), volume changes, Young's modulus (Instron 3369 quasi-static test device), Poisson's ratios in all orientations (3d digital image correlation) and the length of time for samples to return to their unprocessed mass as water leaves the cells is reported in this work. Findings will allow researchers and commercial manufacturers of protective equipment to fabricate and test auxetic closed cell foams.



**Figure 1.** Steam processing conversion method for closed cell auxetic foam.

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# Structures and auxetic material with negative stiffness

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Some mechanical systems and structures under displacement-control loading can exhibit apparent negative stiffness. This phenomenon manifests itself as stress reduction associated with the strain increase. Such structures include rotating levers and non-spherical grains, inverted pendulum and planar topological interlocking assemblies. We discuss the mechanisms of the negative stiffness phenomena. We then consider the dynamics of chains of negative stiffness elements and formulate the conditions of stability of and wave propagation in such chains. We also discuss the stability of an isotropic material with positive Young's and negative shear moduli. Such a material becomes super-auxetic, characterised by the Poisson's ratio smaller than  $-1$ .

Negative stiffness structures and materials only exist as a part of an encompassing system sufficiently stiff to make the total elastic energy positive definite. The investigation of such systems will shed the light on the mechanics behind the structural instability, failure and localisation in engineering and natural materials and structures.



# Designing new auxetic structures based on known 2D systems

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During the past 40 years, a large variety of mechanisms have been devised in order to create structures that are able to exhibit a negative Poisson's ratio [1-8]. However, most of the proposed designs are two dimensional, meaning that in the third dimension the structure is either ignored or still behaves in a conventional way. While this has created a wealth of structures that can find various applications, confining auxeticity to two dimensions restricts the ability of controlling the mechanical properties in the third dimension. This trend appears to have been changing in recent years, with an increasing number of structures showing negative Poisson's ratio in three dimensions being proposed [9-12]. In this context, this work aims at presenting some of the recent progress made in this direction. A variety of structures will be discussed showing how it is possible to use a known auxetic 2D system to build a 3D one.

The work will also present a case study of the deformation of the square grid and its generalisation for large strains and it will be shown that the structures can be designed to attain an incremental Poisson's ratio which is negative for relatively large strains.

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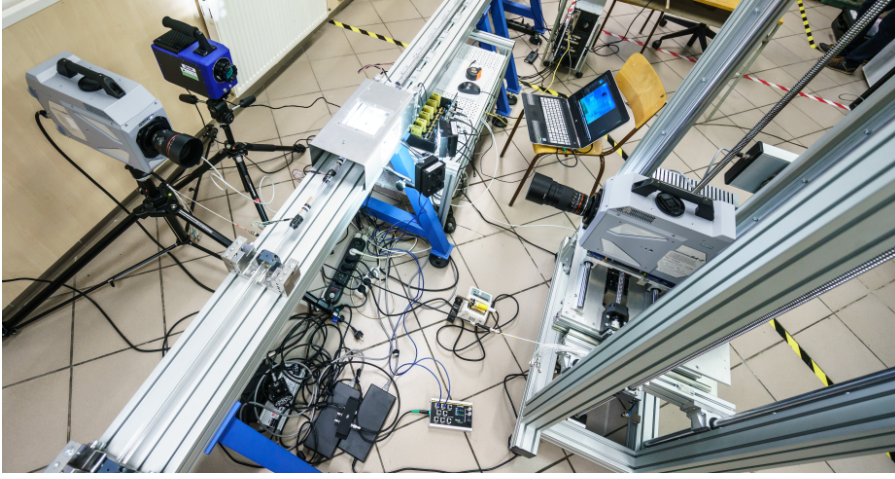
# Strain-rate sensitivity of 316L-0407 steel selective laser sintered auxetic lattices

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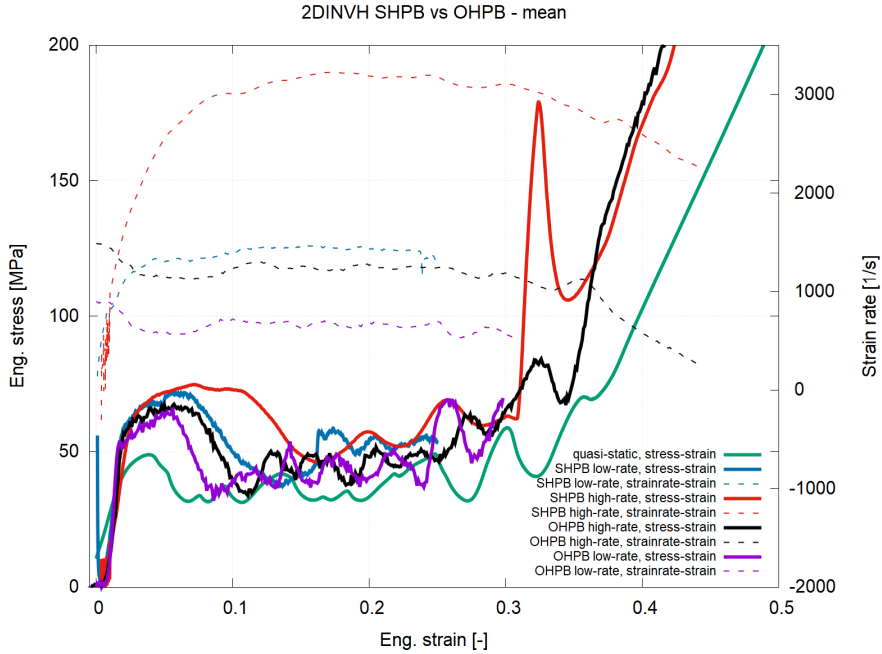
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In this work, selective laser sintered (SLS) auxetic lattices printed from the powdered 316L-0407 austenitic steel were subjected to compressive loading at several strain-rates. Three types of the auxetic lattices were tested: i) 2D re-entrant honeycomb, ii) 2D missing rib, and iii) 3D re-entrant honeycomb. Nominal dimensions of the specimens were approximately  $12 \times 12 \times 12.5$  mm. Due to the optimal printing process, nominal thickness of the individual struts in the lattice was approximately 0.3 mm. Configuration with  $6 \times 6$  cells was used for the 2D structures and  $6 \times 6 \times 7$  cells for the 3D structure. The structures were subjected to the quasi-static uni-axial compression using a standard electromechanical loading device (Instron 3382, Instron, USA) at strain-rate of approximately  $0.0006 \text{ s}^{-1}$ . The experiments were observed using a CCD camera (Manta G-504B, AVT, Germany). In dynamic experiments, the specimens were compressed at four different strain-rates (approximately  $500 \text{ s}^{-1}$ ,  $1200 \text{ s}^{-1}$ ,  $1400 \text{ s}^{-1}$ , and  $3000 \text{ s}^{-1}$ ) using two Hopkinson bar techniques. The experiments at two lower strain-rates were performed using the direct impact Hopkinson bar method with the instrumented incident bar - so called Open Hopkinson Pressure Bar (OHPB). The experiments at two higher strain-rates were conducted using the conventional Split Hopkinson Pressure Bar (SHPB) experimental setup with pulse-shaping technique. All dynamic experiments were observed using a high-speed camera (Fastcam SA-5, Fastcam SA-Z, Photron, Japan) at frame rate ranging from approximately 130 kfps to approximately 250 kfps depending on the impact velocity. An overview of the OHPB experimental setup is shown in Figure 1. Data recorded by the strain-gauges mounted on the measurement bars were used for evaluation of the mechanical behavior of the specimen (e. g., stress-strain and strain-rate-strain diagrams). A custom digital image correlation (DIC) tool based on Lucas-Kanade tracking algorithm was used for the advanced analysis of the displacement and strain fields in the specimens of both quasi-static and dynamic experiments. At least 5 specimens of the each structure were tested per one strain-rate to ensure a sufficient statistics and relevancy of the results.



**Figure 1.** Overview of the OHPB experimental setup with measurement bars and high-speed cameras.



**Figure 2.** Stress-strain and strain-rate-strain diagrams of the 2D re-entrant honeycomb auxetic lattice exhibiting strong strain-rate sensitivity. Solid lines represent stress-strain diagrams corresponding to the strain-rates represented by dashed lines of the same color.

Experiments of all tested structures were valid and good dynamic equilibrium conditions were observed in the impact experiments. Results from both OHPB and SHPB methods were in very good agreement indicating the same boundary conditions in the impact experiments (e. g. friction effects on the bar-specimen interface). Significant strain-rate sensitivity of the structures was identified as well as the changes in the deformation behavior related to strain-rate effects. As the representative example of the results, the stress-strain diagrams showing the strain-rate sensitivity of the 2D re-entrant honeycomb structure are presented in Figure 2. Representative DIC results are also presented in this work. In our other study, the image data from quasi-static and SHPB experiments were processed using DIC and strain dependent Poisson's ratio of the individual structures was calculated using different methods. It was found out, that the Poisson's ratio of the structures is not only strain dependent but, for some types of the tested structures, it is also strain-rate dependent [1]. To conclude, a complex overview of the deformation behavior of the SLS auxetic lattices manufactured from the 316L-0407 austenitic steel at quasi-static loading conditions and at moderate and high strain-rates is provided in this study. Three types of the lattices were successfully tested and the behavior of the investigated structures was found to be strain-rate sensitive. Deformation behavior as well as the energy absorption related properties at different strain-rates were evaluated and are summarized in the contribution.

## Acknowledgements

The research has been supported by Operational Programme Research, Development and Education in the project INAFYM (CZ.02.1.01/0.0/0.0/16\_019/0000766) and by the Czech Science Foundation (project no. 19-23675S). All the financial support is gratefully acknowledged.

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# The mechanical properties of high pressure ice polymorphs with particular emphasis on their auxetic potential

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H<sub>2</sub>O is one of the most abundant substances found on Earth making up about 70% of the Earth's surface and one of the most common molecular species present in the universe [1]. H<sub>2</sub>O has a rich phase diagram which is dominated by the polymorphs ice VII, ice VIII and ice X in the high pressure, low temperature region. Under such extreme conditions, a number of intriguing phenomena have been observed, such as the transition of molecular ice VIII to the non-molecular symmetric ice X [2,3] when the former is subjected to a high external pressure. Detailed characterization of the properties of the high pressure polymorphs would enable scientists to better understand these systems under such extreme conditions, which is particularly important in the fields of planetary science, chemistry and physics.

In view of the above, the structure and mechanical properties of ice VIII and ice X have been studied through DFT simulations employing GGA-PBE and GGA-PBE-TS for ice X and ice VIII respectively. In order to benchmark the methodology employed, the simulated structures and properties of ice VIII and ice X were compared to the experimentally derived properties, where it was shown that the functionals employed give results which show significant agreement with previous studies.

The elastic constants of these phases were then determined through DFT simulations employing the aforementioned functionals, utilising the constant strain method. The results obtained have shown that ice VIII and ice X have the potential of exhibiting a negative Poisson's ratio, with auxetic potential being predicted for ice X at 45° off-axis in all three major crystallographic planes, while ice VIII exhibits a negative Poisson's ratio on-axis in the (001) plane. Studying the deformation of two orthogonally interconnected rhombi has shown that this predicted negative Poisson's ratio can be attributed to the interplay between dilation and hinging of the rhombi. Moreover, it has been shown that the auxetic potential of these ice polymorphs increases with an increase in hydrostatic pressure, which behaviour is explained by the rhombi approaching quasi-perfect behaviour resulting in a decrease in the distortion of the projected rhombi and an increase in hinging mechanism.

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# Engineering design and characterisation of helical auxetic yarns

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Auxetic materials exhibit negative Poisson's ratio which is of interest for many applications, and textile yarns can be made to have auxetic behaviour, then this research aims to create and evaluate helical auxetic yarns with optimal structural parameters. The quality of the helical yarn is the first important consideration during the manufacture process. The research concentrates on achieving the yarn quality and the auxeticity by studying the effect of helical angles, diameter ratio, as well as binder filament feeding in order to optimize the manufacturing process. The maximum negative Poisson's ratio of the optimized auxetic yarn can be achieved as low as  $-9.6$  with a helical angle of around  $14^\circ$  on average by adopting the optimal procedures on the hollow spindle spinning machine. The optimization of the parameters enabled high quality auxetic yarns to be made with a wider machine's settings. In parallel, theoretical and numerical studies have also been carried out to assist the engineering design of auxetic yarns, and have enabled the comparison between the experimental and geometric calculations. Helical auxetic yarns have also been used to produce woven fabrics for their potential applications in filtration and impact protection.



# X-ray scattering from LC polymers: implications for auxetic response

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It is known that x-ray scattering from non-crystalline organic polymers typically shows a strong peak centered around 4.5 Angstroms. This peak has been assigned to scattering from the carbon atoms in the polymer chain and reflects the interchain distance between adjacent chains. We have used x-ray scattering to investigate the potential for auxetic response in main-chain liquid crystalline polymers having a transversely attached rod. The concept is that, due to the specific nature of the chemical connectivities in these polymers, under extension these rods will rotate to a position oblique to the extended main chain thereby resulting in macroscopic expansion normal to the stretching direction. X-ray diffraction is a useful technique to probe this idea since an increase in interchain distances should accompany this extension.

The fiber specimens were prepared by rapid pulling from a nematic liquid. We anticipate that as the fiber is formed, the polymer chains extend and the transverse rods rotate. Rapid cooling in air takes the fibers quickly below the glass transition of the polymer freezing in the rod orientation. Comparison with the x-ray scattering from the same unoriented polymers allows a look into the changes, if any, in the interchain peaks. In this way it should be possible to infer directly whether the rod rotation - requisite for auxetic response - has occurred. A series of polymers were examined with differing levels of incorporation of transverse rods.

It is seen that with the fibers there is a clear shift in peak maximum to smaller  $2\theta$  corresponding to a larger (interchain) distance and a change in peak shape as well. The peak shape shows a significant sharpening of the peak with a decrease in the shorter interchain distances in the fiber. This is consistent with disruption of the 'snuggled' close packing arrangement in the unperturbed powder form; i.e., rod-reorientation of the transverse rod in the fiber which is trapped in its rotated configuration in the quenched LC glass.

We feel that we have demonstrated the validity of this approach for eliciting auxetic response in this type of polymer and offer suggestions for additional synthetic targets and for the experiments and conditions to further exploit this concept.

# Negative mechanical behaviour

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‘Mechanical metamaterials’ is now a widely accepted scientific term used to describe ‘engineered systems that exhibit macroscopic thermo-mechanical properties that emerge due to the structure of their subunits rather than the specific materials composition’. In these systems, ‘mechanics’ is more important than ‘chemistry’ and thus, very often, they are considered as mere mechanical systems specifically designed to exhibit anomalous macroscopic properties such as zero or negative ratios (e.g. auxetic), moduli and/or indices. Such zero/negative properties are not normally manifested by their conventional counterparts and may thus potentially be used in applications where typical materials cannot. This presentation looks at some of the more recent developments made by the University of Malta group in this field.

# Boron arsenate: an old material with newly discovered 'negative' properties

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Boron arsenate ( $\text{BAsO}_4$ ) is a  $\beta$ -cristobalite-like crystalline material belonging to the  $I\bar{4}$  group which is well characterised and known to be stable and at ambient conditions. It was first characterised by Schulze in 1933 who reported it as a white powder and also reported its crystal structure which was determined by X-Ray crystallography. This work re-examines  $\text{BAsO}_4$  through extensive density functional theory (DFT) based simulations aimed at elucidating the nanoscale deformations that such crystals undergo when subjected to hydrostatic pressure, uniaxial stretching or compression, or shearing. Amongst other things, we report how this material (i) achieves the counterintuitive property of negative linear compressibility (NLC) in the crystallographic  $c$  direction and (ii) exhibits negative Poisson's ratio (NPR) in its (001) plane. We also show how NPR results in enhanced compressibility due to what can be termed as the 'Poisson's ratio strain amplification' effect, a phenomenon that had previously gone unnoticed.

# Single trajectory viscosities of model simple liquids by Molecular Dynamics simulations.

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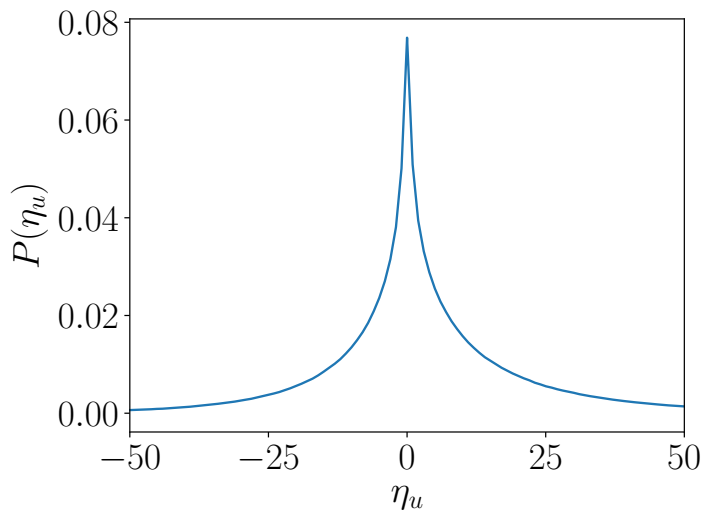
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There are two well-established methods for determining the transport coefficients of model liquids using Molecular Dynamics (MD), the Green-Kubo (GK) time correlation function approach, and by formal rearrangement, the Einstein-Helfand method. We present a third route which is also exactly derivable from GK. In this treatment the (Newtonian) shear viscosity,  $\eta$ , is expressed as the first moment of a probability distribution function or PDF denoted by  $P$  of what we call a ‘single trajectory viscosity’, (STV) or  $\eta_u$ , which is defined as

$$\eta_u = \frac{V}{k_B T} \lim_{t \rightarrow \infty} \sigma(0) \int_0^t \sigma(x) dx, \quad \eta = \int_{-\infty}^{\infty} \eta_u P(\eta_u) d\eta_u, \quad (1)$$

where  $V$  is the volume of the system,  $T$  is the temperature and  $k_B$  is Boltzmann’s constant. The instantaneous shear stress of the liquid at an arbitrary time declared to be zero is  $\sigma(0)$ , and  $\sigma(x)$  is the shear stress at a later time,  $x$ . Note there is no ensemble averaging in the definition of  $\eta_u$  in Eq. (1). The ensemble averaging enters through the second equation in Eq. (1) (i.e., the first moment of  $P$ ). There is no shear rate imposed on the system. Unlike the viscosity itself,  $\eta_u$  can be negative. In fact the probability of  $\eta_u$  being negative is almost as great as it is of being positive. The PDF of  $\eta_u$  is almost symmetric about  $\eta_u = 0$ , and has a large negative stress region. The ratio of the positive to negative sides of the PDF for the same  $|\eta_u|$  varies as  $\exp(A|\eta_u|)$ , where  $A$  decreases to a positive limiting value with increasing  $t$ . The advantage of this third way of calculating,  $\eta$ , is that (a) it provides new insights into the statistics of the dynamical processes which determine the overall viscosity, and (b) the PDF definition of  $\eta$  lends itself to its implementation in coarse grained stochastic approximation models of viscous flow on the nanoscale. For further details see Ref. [1]. Figure 1 shows an example of  $P(\eta_u)$  obtained by MD for a near triple point Lennard-Jones liquid.



**Figure 1.** The STV probability distribution function from an equilibrium Molecular Dynamics simulation.

## Acknowledgements

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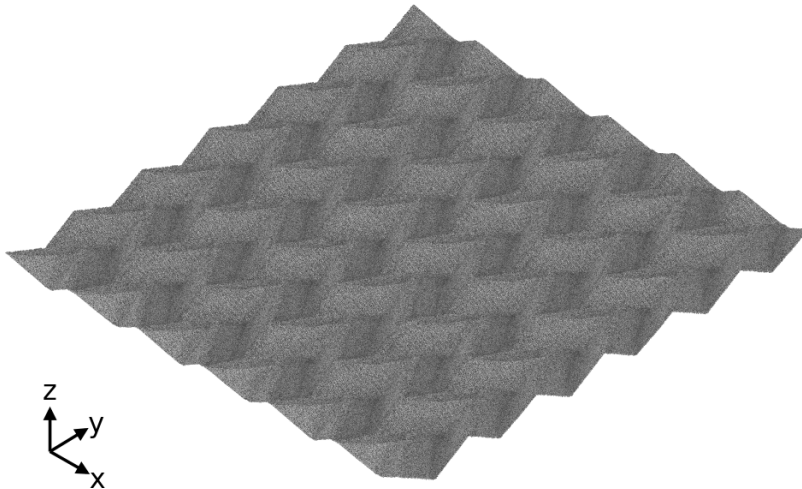
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# An atomic study on mechanical properties of graphene Miura-ori structures

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Origami technique, which is the art of folding paper of some East Asian cultures, is now applied in science and technology [1,2]. Previous studies show that the Miura-ori structure, a smart structure that exhibits excellent mechanical properties including critical bistability [3] and auxeticity [4]. In this study, we use atomistic simulations and density functional theory calculations to study mechanical properties of graphene Miura-ori structures. First, our simulation results show that these structures with a three-dimensional form are obtained by utilizing surface hydrogenation of initial graphene sheets (see Fig. 1). We show that the transformation from an initial sheet to a three-dimensional structure owing to presence of pseudo surface stresses induced by the surface functionalization. Then, we find that these graphene structures exhibit simultaneously excellent mechanical properties including auxeticity, super-compliance, and super-flexibility. Finally, we show that the mechanical properties are readily tailored by controlling the surface functionalization.



**Figure 1.** A graphene Miura-ori structure obtained by the surface hydrogenation.

## Acknowledgements

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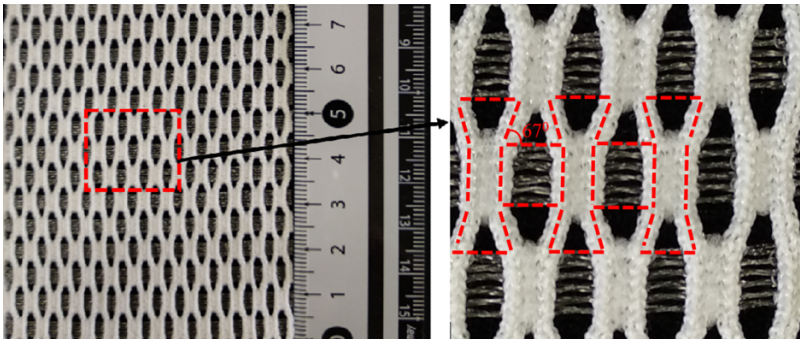
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# Deformation behaviour of warp knitted fabric made with re-entrant hexagonal geometry

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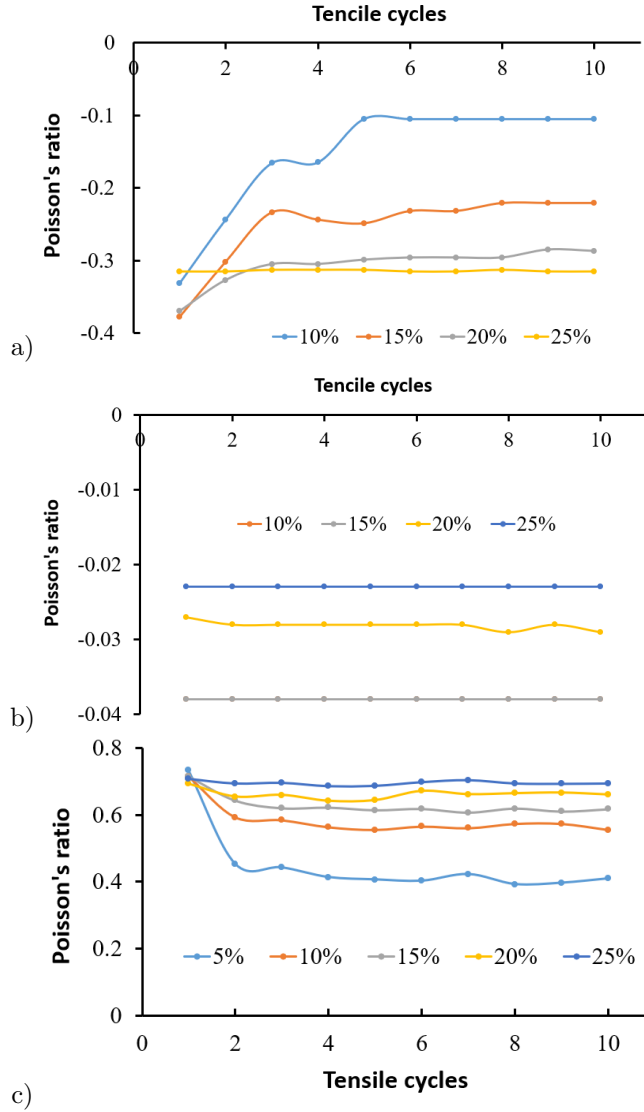
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Auxetic warp knitted fabrics made with re-entrant hexagonal geometry have been designed and studied in our previous work in terms of its auxetic behaviour in different directions and the knitting parameters that could affect the auxetic effect of the fabrics. The results showed that the fabric proposed could have good auxetic effect under single tension in either wale direction or course direction. However, the behaviour of these fabrics under repeating tension test is still unknown, which is quite necessary for the daily use, because most of them will not be used as disposable ones and they are supposed to be subjected to repeat tension. Therefore, this research aims to study the auxetic behaviour of the fabric (Fig. 1) under repeat tension. All the samples were tested with 100 times of loading in the wale direction, the course direction and the diagonal direction which has a  $45^\circ$  to the former two directions. During the test, each fabric sample was firstly stretched to a strain of 25% and then held for 2 seconds before releasing the tension. After the fabric sample had returned to its original size, 10 seconds were given to the sample for relaxing before the next circle of tension. According to the results, no auxetic effect was observed when tested in diagonal directions (Fig. 2c). However, after several times of stretch, all the fabric samples show good resilience, and the auxetic effect in wale direction and course direction becomes stable (Fig. 2a and 2b). Even after 100 times of stretch, the fabric samples can still have auxetic effect in the above two directions. The results show that the auxetic warp knitted fabrics based on re-entrant geometry can keep good auxetic effect under repeating tension especially in wale direction and they might be used as auxetic materials in repeating tension conditions.



**Figure 1.** Warp knitted fabric made with re-entrant geometry.





**Figure 2.** Auxetic behaviour under repeating tensile conditions a) wale direction, b) course direction and c) diagonal direction.

## Acknowledgements

The authors would like to thank the funding support from the Research Grants Council of Hong Kong Special Administrative Region Government (grant number: 15209616).

# Temperature-tuneable auxetic structures

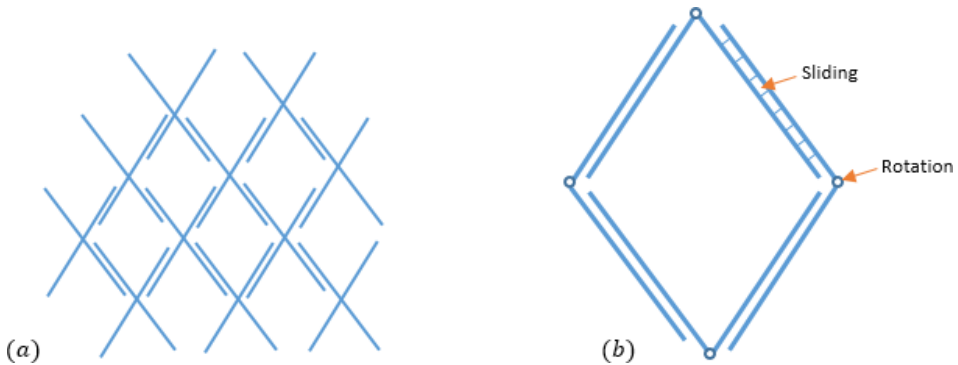
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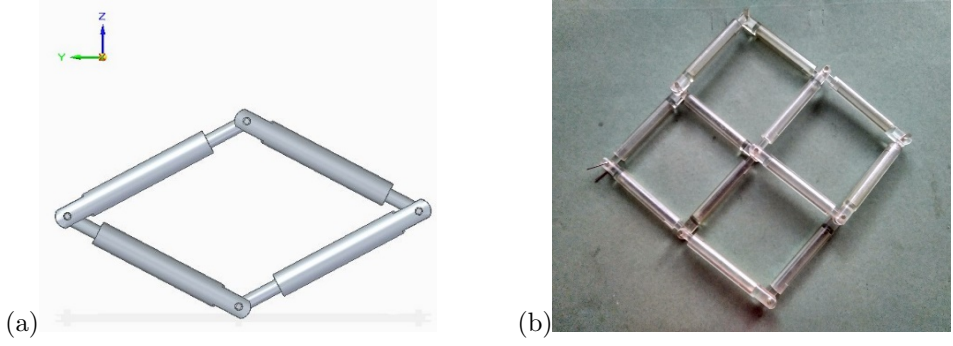
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Simple two-dimensional structure presented here with tuneable auxetic behaviours. The structure has rotating and sliding elements (see Fig. 1), where the sliding part can be switched on/off by using an external temperature field. When the sliding is “off”, the structure is non-auxetic, while when it is “on”, it is auxetic. The easiest way to realize this behaviour is to fill the gap between the piston and cylinder parts of the sliding unit with a lubricant showing glass-transition in a certain temperature range. When the lubricant is in normal liquid state, the sliding parts move almost freely with  $\nu = -1$ ; it is called the “free sliding, no rotation” state. By reaching the glass transition, the extremely high viscosity of the lubricant stops sliding and the structure can be deformed only through the rotating units; this is the so-called “no sliding, free rotation” state, where  $\nu > 0$ .



**Figure 1.** (a) Full structure. (b) Elementary unit of a rhombus-shape structure with sliding sides and rotating vertexes.



**Figure 2.** Design of the elementary cell (a) and a 4-unit part, produced with 3-D printing (b).

Theoretically one can create continuous transition between the low-viscosity and high viscosity states of the lubricant, but with normal liquid, the two extrema would not be reachable, therefore presently we are studying only these two cases. 3-D printed model of the structure can be seen in Fig. 2.

# Double-negative metamaterial structures analysis

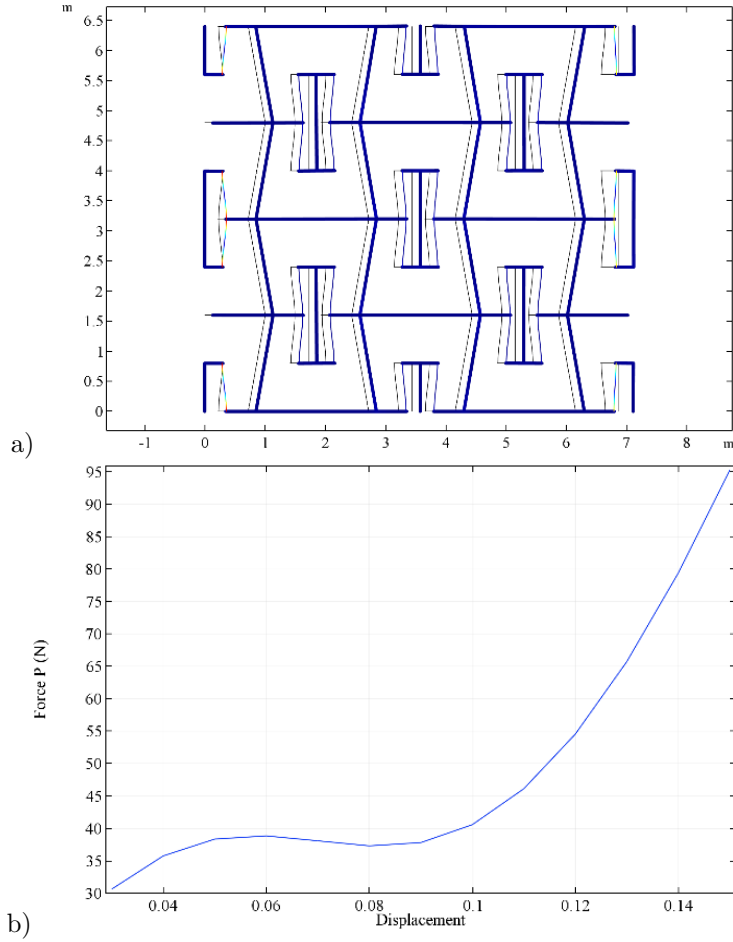
H. Jopek<sup>1</sup>, O. Duncan<sup>2</sup>, and A. Alderson<sup>2</sup>

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<sup>2</sup> *Sheffield Hallam University, Sheffield, United Kingdom*

Linear elasticity based on the constitutive generalized Hooke's law is widely used in modelling of numerous mechanical systems. However, a linear relation between the force applied and displacement is typically valid only for a small range of deformation. Above a certain level of strain (usually not more than 10%) nonlinear models are required in order to appropriately represent the deformational behaviour of the material system. The nonlinearity is a result of material mechanical properties but it could also results from the specific geometry of the considered system. In fact, both conditions can interact, especially when considering the microstructure of materials and its impact on the effective properties of materials. In particular, the relation between the force and displacement could be not only nonlinear but also non-monotonic i.e. one can observe the increase of the displacement while the force acting on the mechanical system is decreasing. Such behaviour is called a negative stiffness.

This research was focused on the possibility of creating novel two- or three-dimensional double-negative structures i.e. structures characterized by negative stiffness and negative Poisson's ratio. Both negative stiffness and auxeticity (negative Poisson's ratio) are very unusual, therefore structures which combine both of these properties are even more exceptional. So far, few examples have been studied [1] for the two-dimensional case. All simulation by means of FEM method was performed with the use of Comsol Multiphysics Software.



**Figure 2.** a) Exemplary modified auxetic structure, b) Force vs displacement plot.

## Acknowledgements

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# From Cauchy to Willis continuum

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We will discuss the Willis equations (also known as Milton-Briane-Willis equations) as a generalization of Cauchy continuum mechanics to describe chiral elastic media. We will explain how it can qualitatively describe recent static experiments on 3D chiral cubic-symmetry metamaterials by introducing a single additional parameter, linked to a local scale, with respect to Cauchy elasticity. This approach is an alternative to Eringen continuum mechanics (or micromorphic), in which nine (six) additional parameters appear.

# Undulation instability and kink formation of layered block copolymers: a coarse-grained molecular dynamics study

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The properties of plastic deformation in solids are typically sensitive to their nano- and microstructures. In particular, various layered solids exhibit a high degree of anisotropy, i.e., there is a significant difference between properties parallel to the layers and those perpendicular to them. Exploring the mechanical characteristics of such “mille-feuille-like” microstructures with alternate hard and soft layers provides potential insights for developing new structural materials.

When thermoplastic elastomers in an aligned lamellar or hexagonal morphology are stretched perpendicularly to the plates or rods, the lamellae or cylinders buckle to form a chevron or zig-zag structure above a critical stress [1-3]. As has been reported by Cohen et al. [1,2], polystyrene/polybutadiene (PS/PB) lamellae in a styrene-butadiene-styrene (SBS) triblock copolymer oriented perpendicular to the tensile direction can deform via bending of the lamellar normal out of the deformation axis. This nucleates a kink band from which the kink boundaries can propagate parallel to the deformation direction. This causes undulation of adjacent regions until the entire structure is turned into a chevron structure.

In this study, we investigated the onset of undulation and the resultant kink formation in layered triblock copolymers using a coarse-grained molecular dynamics approach. Coarse-grained models of microphase-separated lamellar copolymers with alternate glassy (hard) and rubbery (soft) layers were constructed based on the bead-spring model [4-6] in combination with the dissipative particle dynamics method [7,8]. For sufficiently large systems, oriented block copolymers exhibit a buckling instability due to the Poisson contraction of the hard layers when submitted to a tensile test perpendicular to the lamellae direction. The buckling, which led to tilting and undulation of the layers, was associated with a sharp turnover in the stress-strain curve and the plateau level of the stress was related to the microstructural transition to the kink morphology. Consequently, the layers evolved into the chevron-like shape on further strain beyond the instability. We found that the deformation behavior strongly depends on temperature relative to the glass-transition temperature of both phases. The amount of glassy (hard) phase was larger and before undulation of the lamellae was observed, catastrophic crazing (or cavitation) in the soft layers occurred. The results suggested that the deformation mechanism of layered block copolymers was dominated by the competition between the buckling of the hard layers and the cavitation in the soft layers during elastic deformation.

## Acknowledgements

This work was supported by a Grant-in-Aid for Scientific Research on Innovative Areas (Grant No. A18H054800) from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan.

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# Thermoelastoplastic analysis of reentrant cell formation

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Effective Poisson's ratio of foam is negative when its cell shape is reentrant. A method to convert the initially convex cell shape, which gives rise to positive Poisson's ratio, to the reentrant one is through the thermal transformation technique for polymeric foam. Conventional metal foam may be converted to exhibit negative Poisson's ratio by plastic deformation, without heat treatment. In this work, we numerically investigate the formation of reentrant cell shape from the state of near hexagonal shape in two dimensions. The theory of thermoelastoplasticity with large deformation is adopted. Based on the chosen parameters used in our finite element calculations, effective Poisson's ratio of about -0.5 is achieved in the infinitesimal strain range. Under large straining, the effective Poisson's ratio of the 2D foam gradually becomes positive. The loss of auxeticity in large deformation is due to the loss of reentrant geometry in the cells. In addition, effects of residual stress on auxeticity will be discussed.

# Nonclassical properties in heterogeneous solids

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Lattices based on rib elements (truss lattices) and plate elements (plate lattices) offer design freedom in which physical materials can be embodied via 3D printing. Properties such as negative Poisson's ratio, tunable thermal expansion, and tunable piezoelectric response are attainable via designed lattices. Such lattices do not obey the classical theory of elasticity. Deviations from classical response can be understood in the context of generalized continuum theories such as couple stress theory, Cosserat elasticity, void elasticity or nonlocal elasticity. Predictions of generalized continuum theories include size effects in torsion and bending, alteration of stress concentration factors, changes in strain distribution, and changes in wave propagation. Generalized continuum aspects of cellular solids including truss lattices, with experimental demonstration of effects, will be discussed.

# Auxetikos (αυξητικός) systems

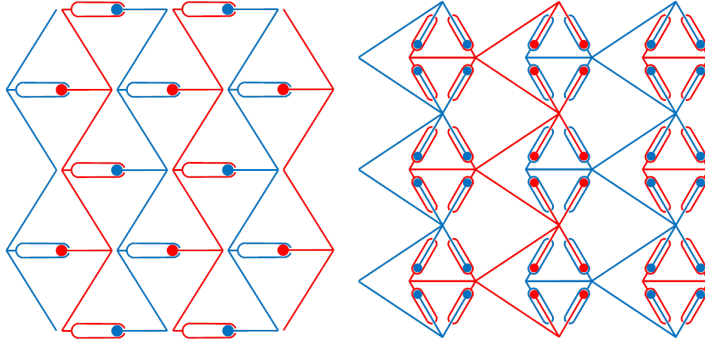
T.-C. Lim

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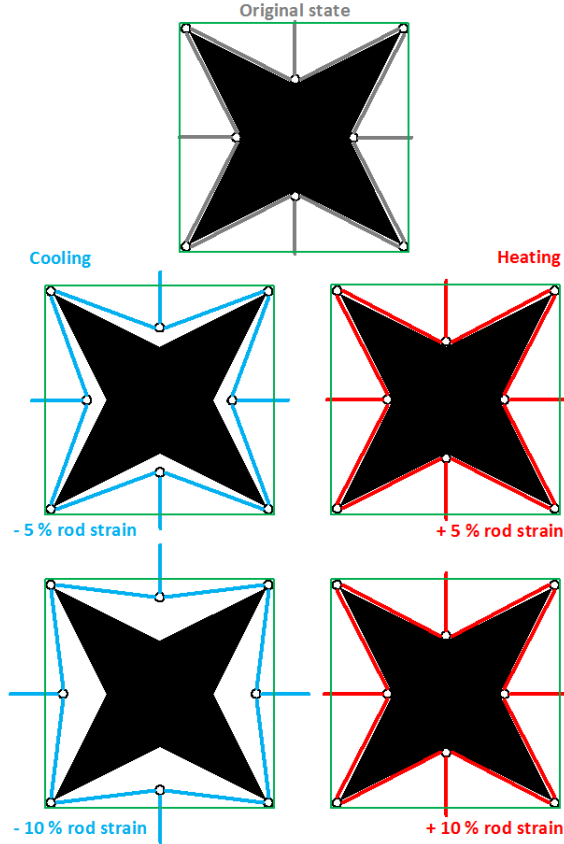
The term “auxetic” is defined as “negative Poisson’s ratio”. This is derived from its root word in Greek “αυξητικός” (auxetikos), which means “that which tends to increase”. The concept of auxetikos systems is introduced herein by means of in-situ sign-switching of material properties such that strain is always positive in response to applied stimuli, i.e.

$\nu_{ij} > 0$  (non-auxetic) when  $\sigma_{ii} < 0$  but switches to  $\nu_{ij} < 0$  (auxetic) when  $\sigma_{ii} > 0$   
such that  $\varepsilon_{jj} > 0$ , and  
 $\alpha > 0$  (PTE) when  $dT > 0$  but switches to  $\alpha < 0$  (NTE) when  $dT < 0$  such that  
 $\varepsilon_{ii} > 0$  and  $\varepsilon_{jj} > 0$ .

The 2D examples used herein employ microstructural duality, i.e. every microstructure is architected in such a manner that two distinct effective microstructures exists, whereby each effective microstructure takes turn to manifest itself under opposing stimuli. This duality is effected by introducing redundant parts to co-exist alongside the functional parts for a particular stimulus. Under an opposing stimulus, the functional and redundant parts are rendered redundant and functional, respectively. Figure 1 (left) shows the hybrid rhombic-re-entrant microstructure, which functions as re-entrant microstructure under horizontal tension but becomes rhombic microstructure under horizontal compression, while Fig.1 (right) shows a hybrid kite-arrowhead microstructure, which is effectively a double-arrowhead microstructure under horizontal tension but switches to kite microstructure under horizontal compression. Therefore, under the action of either tensile ( $\sigma_{xx} > 0$ ) or compressive ( $\sigma_{xx} < 0$ ) axial loads, the transverse strain is always positive  $\varepsilon_{yy} > 0$ , i.e. the transverse dimension tends to increase. Figure 2 illustrates an interconnected shuriken network with pin-jointed PTE rods. Upon cooling all rods contract but upon heating only the horizontal and vertical rods expand because the inclined rods are locked in place and are therefore non-functional. For this reason, under the influence of thermal fluctuation the thermal strains are always positive, i.e. the in-plane dimensions *tend to increase*.



**Figure 1.** The hybrids of rhombic-re-entrant (left) and kite-arrowhead (right) microstructures.



**Figure 2.** A unit cell of the rigid shuriken network, with pin-jointed PTE rods in its original state (top row) undergoing cooling (left) and heating (right); the rods encounter thermal strains of  $\pm 5\%$  (middle row) and  $\pm 10\%$  (bottom row). Green boxes = original dimensions.

# Tension of thin two-layered plates and nano/microtubes of hexagonal crystals

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The problems of stretching two-layered plates and nano/microtubes of hexagonal crystals are considered. Analytical formulas for effective Young's modulus and effective Poisson's ratio of two-layered composites of hexagonal crystals are obtained. The effective elastic properties (Young's modulus and Poisson's ratios) of the plate are dependent on the properties of the components of the plate's crystals, such as the sign and magnitude of Poisson's ratios, the ratio of Young's moduli, and the ratio of layer thicknesses. A numerical analysis of the elastic properties of two-layered composites was performed. It is shown that the presence of an auxetic layer can lead to a violation of the rule of mixtures. However, for small differences in Young's modulus and Poisson's ratios of the initial crystals, prediction accuracy of effective Young's modulus by the rule of mixtures it turns out to be quite satisfactory.

## Acknowledgements

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# Analytical and Finite Element modelling of crystalline cellulose $I_\beta$

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Crystalline cellulose  $I_\beta$  obtained from Kraft cooked Norway spruce is known to have a negative Poisson's ratio, thus corresponding to auxetic behaviour [1]. Previous work carried out by Yao et. al. [2] looked at modelling the cellulose  $I_\beta$  using molecular mechanics and developing conceptual models. The work presented at the Auxetics conference in 2018 highlighted analytical models developed based on the molecular mechanics models mentioned above, including a details parametric study.

The work presented here expands on these results as further analytical models developed, including Young's Moduli, will be presented and discussed in line with previous work. Additionally, 3D models based on the 2D analytical models are presented in detail. Finite element modelling results of the 3D models are also discussed, thus providing a comprehensive understanding of the auxetic behaviour obtained in the system.

## Acknowledgements

This work is supported by a match funded Vice Chancellor's Scholarship Scheme in the Materials and Engineering Research Institute at Sheffield Hallam University, in collaboration with Michelin.

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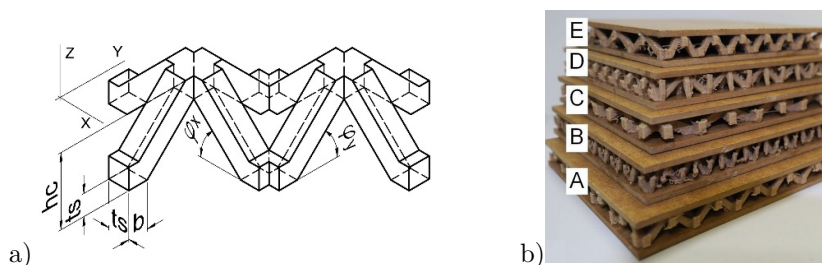
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# Experimental testing of elastic properties of laywood pyramidal cores

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In the furniture industry, the most commonly used cellular boards are light furniture boards made of paper core with hexagonal cells. In case of using lattice and pyramidal structures from wooden composites to produce the core structure of sandwich boards [1], it should be noted that these works are few and aimed mainly at determining the elastic properties of such structures [2,3]. The geometry of cores with the pyramidal cells and different types of outer layers wood materials has been investigated. The aim of the research was to determine the effect of the pyramidal geometry of the lattice core cell on the mechanical properties of a light board panels (Fig.1). An analytical model of the pyramidal cell was developed and studies were conducted to determine the effect of pyramidal core geometry on the mechanical properties of the core while maintaining similar relative density values. Then, it was decided to perform FEM analyses of the selected structures, and to compare the results with experimental investigations of cores made in 3D printing technology using the FDM method. To produce the cores, filaments with the trade name LayWood containing wood dust were used.



**Figure 1.** Pyramidal core: a) geometry b) samples.

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# The use of XFEM in the analysis of fracture resistance of auxetic re-entrant cell

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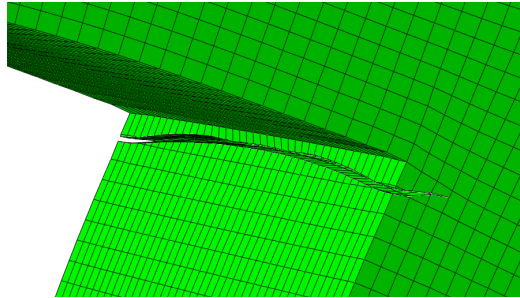
Auxetic materials are recently very popular topic in material science. They exhibit unusual properties because of their negative Poisson's ratio. Mainly their deformation is opposite than in regular materials – they become thicker when subjected to tension and thinner when subjected to compression. However, also the dynamic properties of these materials are different. Fatigue of auxetics is an interesting topic for future works. But in order to fully understand the fatigue behaviour of these new materials, their fracture resistance should be studied first as these two properties are closely related. Currently, there are only a few works about fracture resistance of auxetics giving us a new interesting area of research [1,2,4].

The works performed for this paper consist of two main steps. The first one was to use the Extended Finite Element Method (XFEM) to predict crack location, size, and direction of growth. The second step was to approximate such predicted crack geometry, treat it as stationary and calculate the values of J integral as well as stress intensity factors using XFEM again. These two steps were performed for both hexagonal honeycomb and re-entrant structure to compare their crack resistance. The models were prepared as complementary – they were created by just changing the angle between inclined ribs. Simulations were performed in Abaqus software. The J-integral calculated in this paper is given by the following formula (1) [3,5,6]:

$$J = \int_{\Gamma} \left( W n_1 - T_i \frac{\partial u_i}{\partial x_1} \right) ds, \quad (1)$$

where:  $W$ –strain energy density,  $n_1$ –normal vector,  $T_i = \sigma_{ij}n_j$ –traction vector,  $u$ –displacement vector.

In the below picture (Figure 1) an exemplary crack predicted by XFEM can be observed.



**Figure 1.** One of two cracks predicted for the re-entrant cell.



## Acknowledgments

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# Using auxetic structures for stents

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Natural deformations of the main blood vessels during the cardiac cycle are characterized by simultaneous dilatation and elongation at systole. Changes in mechanical properties of the blood vessels like stiffening have been reported to affect local artery function and global hemodynamics [1]. These can be associated with normal ageing, congenital conditions, or vascular diseases. Although vessel's stiffening is a recognized predictor of cardiovascular events, stents and stent-graft devices commonly used to repair or replace the blood vessels are not currently designed to address this problem and restore the healthy dynamic pattern.

The aim of this study is to develop new stent designs that can replicate the physiological motion pattern of the healthy blood vessel, by using auxetic structures. In particular, our research has focused on three different auxetic cellular configurations that are most suitable for adaptation into tubular structures: the re-entrant hexagonal honeycomb, the double-arrowhead shape and the hexachiral shape [2]. Comparison between the different auxetic configurations has highlighted the different potentiality of each structure for a variety of cardiovascular stent applications. The effect of the possible changes in the characteristic geometric parameters defining each auxetic configuration over the mechanical response of the tubular structure to circumferential expansion, axial tension and twisting was analysed by means of finite element modelling (using the implicit non-linear software MSC.Marc) and analytical descriptions, as a mean of validation.

The study has confirmed that auxetic configurations can enable the incorporation of a healthy physiological dynamics into stents and stent-graphs, contributing to enhance their efficacy by restoring a more efficient function and a reducing the alterations associated with cardiovascular events.

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# Recent progress in modelling of nano auxetics by hard body systems

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Elastic properties of hard body model systems have been determined by Monte Carlo simulations using Parrinello-Rahman method [1-3] in the isothermal-isobaric ensemble. The purpose of the study was to determine the influence of the so-called *nanoinclusions* (composed of identical particles, placed in the matrix of the other type of particles) on the elastic properties and Poisson's ratio [4] and in particular, to search for systems with negative Poisson's ratio [5] (also known as *auxetics* [6]).

The studied models were based on the f.c.c. lattice formed by identical hard spheres of the diameter  $\sigma$  (called the matrix of the system). Into such a structure nanoinclusions were introduced in the form of a periodic array of nanochannels, a periodic stack of nanolayers or the superposition of both. The inclusions were introduced by replacing selected matrix particles by inclusion particles. The latter differ from the matrix hard spheres only in the value of their diameters ( $\sigma'$ ). The channels were oriented in [001]-direction and the layers were oriented perpendicularly to [001]- or [110]-directions.

It is known [7] that f.c.c. structure of hard spheres exhibits partial auxeticity (negative Poisson's ratio in the [110][ $\bar{1}\bar{1}0$ ]-direction). Preliminary research has shown that nanoinclusions in the form of nanochannels [8] and monolayers [9] can constitute an efficient way to decrease the value of Poisson's ratio in certain directions. It has been also shown that a monolayer of hard spheres of the diameter larger than the diameter of matrix spheres ( $\sigma' > \sigma$ ) doubles the negative value of the Poisson's ratio ( $\nu = -0.11$ ), whereas in the case of narrow nanochannels the minimal Poisson's ratio observed was as low as  $\nu = -0.873$ . The data presented in this talk are the results of in-depth study of the influence of such inclusions of different sizes (e.g. wider nanochannels) and under different pressures and orientations (nanolayers perpendicular to [110]-directions). It is shown that such nanoinclusions may be used not only to enhance auxetic properties but also to make the system completely non-auxetic, or to constrain the extreme negative Poisson's ratio to a certain range of possible values.

## Acknowledgements

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# Computational and experimental investigation of fatigue behaviour in re-entrant auxetic cellular structures

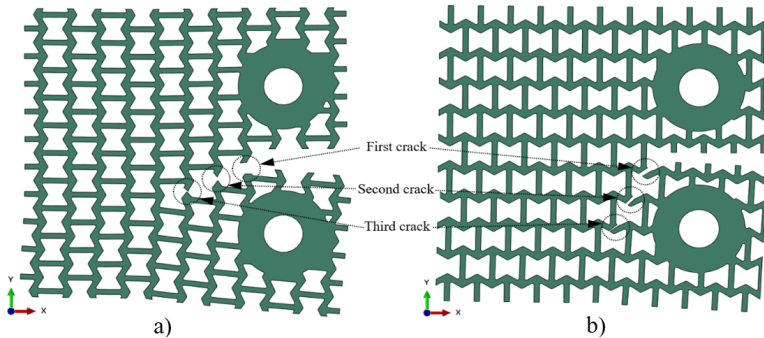
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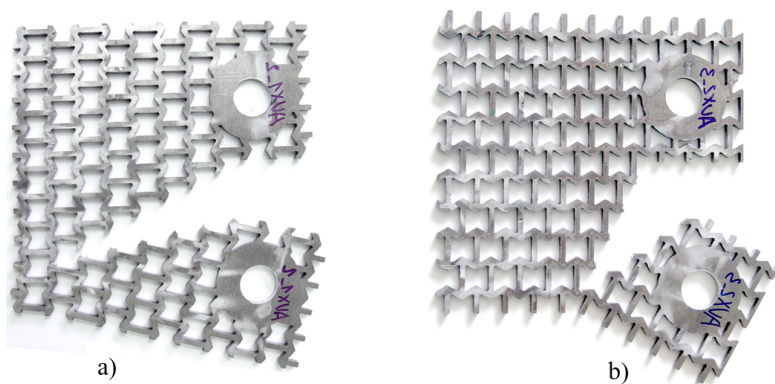
Computational and experimental investigation of fatigue behaviour of auxetic cellular structure made of Al-alloy 7075-T651 is presented in this study [1]. Fatigue investigation of selected auxetic cellular structures were performed in a low-cycle fatigue regime [2], under load control with stress ratio  $R = 0.1$ . In computational investigation, the complete fatigue process of analysed cellular structure is divided into the crack initiation ( $N_i$ ) and crack propagation ( $N_p$ ) period where the total fatigue life ( $N$ ) is defined as [1]:

$$N = N_i + N_p \quad (1)$$

The crack initiation period,  $N_i$ , is determined using the strain life approach in the framework of the FE-Safe computational code, where elastic-plastic computational analysis is performed to obtain the total strain amplitude in the critical cross-section of the analysed structure. The number of stress cycles,  $N_p$ , required for the fatigue crack propagation from the initial to the critical crack length is also determined numerically using a finite element model in the framework of the Abaqus computation FEM code. The Maximum Tensile Stress (MTS) criterion is considered when analysing the crack path inside the cellular structure (Fig. 1). Finally, experimental fatigue tests (Fig. 2) were also performed to validate the computational model. Experimental tests were performed in a low-cycle fatigue regime at the same load level [1,3].



**Figure 1.** Crack paths of treated cellular structures a) Re-entrant auxetic structure (AUX\_1); b) Rotated re-entrant auxetic structure (AUX\_2).



**Figure 2.** Experimentally determined crack paths of treated cellular structure a) Re-entrant auxetic structure (AUX\_1); b) Rotated re-entrant auxetic structure (AUX\_2).

## Acknowledgements

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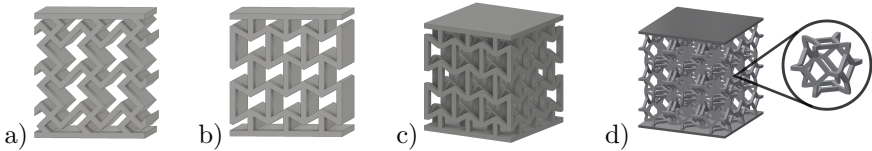
# Numerical modelling of SLS printed auxetic lattices subjected to compressive loading using SHPB

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Split Hopkinson Pressure Bar (SHPB) is an experimental apparatus suitable for investigation of strain and strain-rate dependent properties of auxetic lattices at high strain-rates [1]. To be able to estimate parameters of the SHPB setup for testing of the auxetic specimens, i.e. diameter and length of the individual bars, material properties of the bars, the pulse-shaping technique, the striker impact velocity, etc., and to optimize the properties of the lattices, numerical modelling using finite element (FE) method is an advantageous approach to deal with such tasks [2,3]. However, due to the nature of dynamic effects present during high strain-rate loading such as micro-inertia, mechanical impedance and contact boundary conditions, it is favorable to use full-scale virtual (numerical) representation of given SHPB apparatus. Then, it is possible to perform virtual experiments such that the quantities calculated and evaluated at virtual strain-gauges on a numerical model can be directly compared with the actual experimental data. This enables an immediate verification of the the SHPB parameters estimation and comparison between numerically and experimentally assessed characteristics of the investigated lattice, since the true geometry of the SLS printed sample is used in the simulations, i.e. FE mesh is generated directly from the geometrical model used for the SLS printing procedure.

The main aim of the presented study is to demonstrate FE modelling of various auxetic lattices subjected to compressive loading with the emphasis on transition from quasi-static to high strain-rates. Four different unit-cell geometries were selected for the study: a) missing-rib, b) two-dimensional re-entrant honeycomb, c) three-dimensional re-entrant honeycomb, and d) re-entrant tetrakaidecahedron (see Fig. 1).



**Figure 1.** Visualization of the SLS printed specimens: a) the missing-rib structure, b) the two-dimensional re-entrant honeycomb structure, c) the three-dimensional re-entrant honeycomb structure, d) the re-entrant tetrakaidecahedron structure with a detailed visualization of the unit cell.

To improve reliability of the dynamic simulations, a sensitivity study comprising mesh parameters (element size, mesh generation algorithm) was performed. The virtual specimens were created by a periodical assembly of the unit cells in all spatial directions taking into account limits of the SLS printing device (Renishaw AM250) and computational aspects of the simulations. The numerical models of the specimens were used to perform simulated uni-axial quasi-static experiments using Ansys FE code and dynamic SHPB experiments using LS-DYNA code. The elastic isotropic material model was used for modelling of the bars owing to fundamental requirement on purely elastic behavior of the bars during valid experiments. Different elasto-plastic material models were used for modelling of the specimens to assess their influence on obtained results. Constants of both the material models, of the bars and the specimens, were experimentally calibrated using the SHPB void tests (i.e. SHPB tests without specimen) for calibration of elastic constants of the bars and the uni-axial compression of SLS printed bulk specimens at different strain-rates in case of the auxetic specimens. Hexahedral constant-stress elements were used for numerical representation of the bars, while the mesh of the specimen geometry was generated using: i) linear or quadratic tetrahedral elements in quasi-static simulations and ii) by constant-stress or fully integrated tetrahedral elements in the dynamic simulations. The quasi-static simulations were performed as displacement controlled simulated loading to assess the effective stiffness of the specimens and the yield point of the structure, while self-contact condition was applied on the specimens in the dynamic simulations to be able to evaluate their deformation response up to densification region after multiple passes of the strain-waves. To assess the deformation behaviour of the investigated microarchitectures, compressive stress-strain diagrams and strain-dependent Poisson's ratio at quasi-static and dynamic loading conditions were studied.

## Acknowledgements

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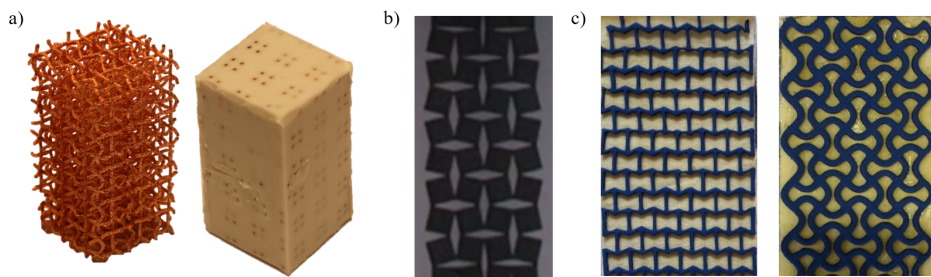
# Towards the stiffer and cheaper auxetic cellular materials

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Auxetic cellular structures are modern metamaterials, which posse negative Poisson's ratio [1,2]. They tend to expand in lateral direction when subjected to tensile loading and vice versa in the case of compression loading. This behaviour is beneficial for many applications, especially in the field of engineering, crashworthiness, ballistic protection, medicine and fashion. In order to use these materials in serial produced practical applications, there is a necessity to reduce the cost of their production, to enhance their stiffness and to improve their properties offering superior advantages in comparison to other materials.

In this work, three different methods and propositions for stiffer and cheaper modern auxetic cellular structures will be discussed. The analysed samples are shown on Fig. 1: a - auxetic structure embedded in silicone, b - rotating squares cuts in nonwoven fabric and c - auxetic textile composites.



**Figure 1.** Hybrid auxetic chiral structure (a), rotating squares structure (b) and auxetic textile composites (c).

The additively manufactured chiral auxetic cellular structures were embedded in silicone (Fig. 1a), resulting in hybrid auxetic cellular, which offers additional support to the auxetic cellular structure during the deformation. This enhances the mechanical properties and postpones the brittle collapse of auxetic structure up to larger strains.

The mechanical and deformation response of needle-punched nonwoven fabric with rotating squares [3] pattern was evaluated (Fig. 1b). This fabric is a synthetic leather used for a heel grip, insole and lining material (in the footwear industry), as well as lining material in the manufacturing of belts. The dependency of stiffness, out-of-plane bending and negative Poisson's ratio was evaluated in this part.

Finally, the auxetic textile composites were evaluated, where the composite consists of cotton fabric and two-dimensional auxetic structure cut from thin foam

sheet (Fig. 1c). The fabric and auxetic structure were bonded with adhesive and tested under tensile loading. It was found that the textile composite provide enhanced mechanical properties. Furthermore, the macroscopic auxetic behaviour can be observed till moderate strains.

As it was shown in the three case studies, the auxetic cellular structures can be fabricated in the way that they are stiffer and/or cheaper. Studies like this are necessary for the future practical applications of novel structures/materials in serial production of modern parts in the field of engineering, medicine and fashion.

## Acknowledgements

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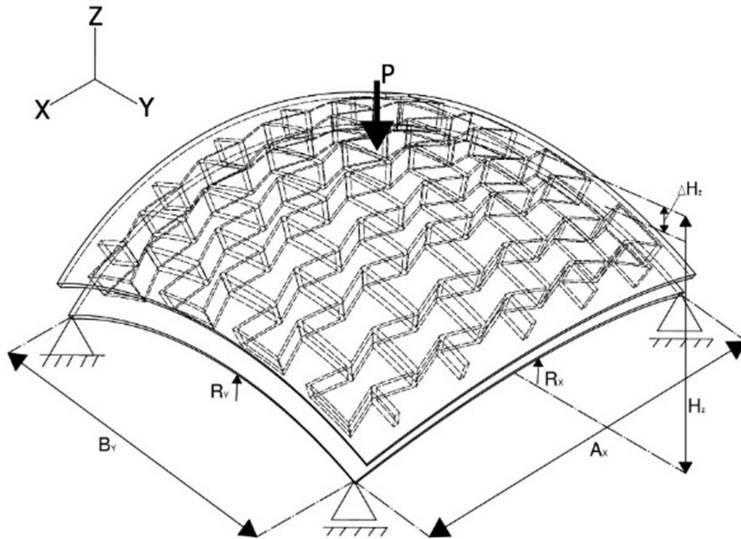
# Usability of wood based auxetic sandwich panels to form synclastic shapes

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Auxetic structures are interesting in terms of improving stiffness and durability of the material [1]. They tend to form synclastic, sphere-like shapes instead of anticlastic curvature which is characteristic for standard materials with positive Poisson ratio, subjected to bending [2].

Nowadays in wood industry, furniture which were designed with use of synclastic shapes, are typically made from bent steel frame (usually upholstered), plastics or bent plywood. Technology of bent plywood is strictly connected with thermo-physical treatment, mold casting and temperature-pressure bending process. The process is both time- and resource-consuming. This situation could be improved by implementation of auxetic structures into the industry [3].



**Figure 1.** Synclastic panels made from novel wood based composites.

In this research authors performed examination of synclastic panels made from novel wood based composites (Fig.1). The aim was to determine stress-strain characteristics during uniaxial compression and obtain stiffness of the panel. Additionally authors measured stress of outer and inner layers occurring during examination. Furthermore MES analysis was performed, to determine influence of technological execution of the samples on the quality of obtained experiment

results. It was demonstrated that proposed novel sandwich type composites allow to form technologically difficult, spherical shapes, without additional treatment of heat and pressure. Type of the outer layer material strictly determines the usability and ease of 2-axis bending process. Presented composites are interesting materials, that could have been implemented into the wood industry as a replacement to traditional materials, such as bent plywood.

## Acknowledgements

The present work was conducted as part of the research project no. UMO-2016/21/B/ST8/01016 financed from the funds of the National Science Centre.

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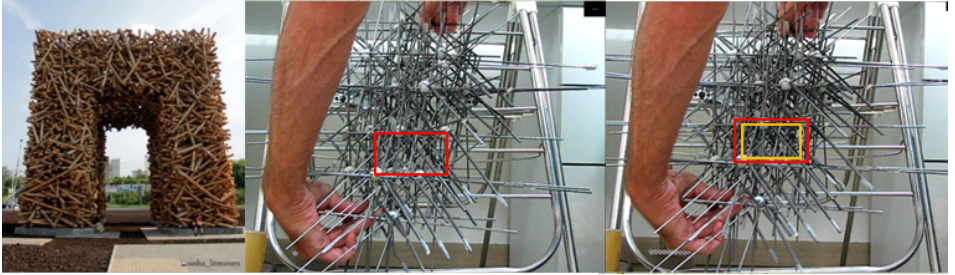
# Entangled straight lines and auxetics

P. V. Pikhitsa<sup>1</sup> and S. Pikhitsa<sup>2</sup>

<sup>1</sup> *Seoul National University, South Korea*

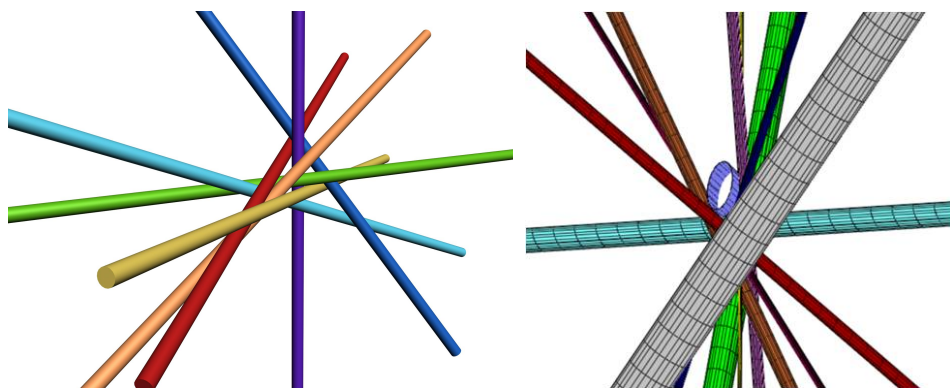
<sup>2</sup> *Odessa National University, Ukraine*

Auxetics are all about constraints, imposed on structural units, mostly the ones that correlate mutual orientations and restrict free motion in 3D. E.g. balls (points) as structural units are least restrictive and may lead to rubber behaviour. On the other pole there are long rods (impenetrable straight lines), the units most prone to jamming and orientation constraints. One may suspect that if our Space were the space of straight lines instead of the space of points, it would be auxetic and could expand in all directions, as it actually does. We discuss entanglement of straight lines in 3D space, that may be relevant to a possible realization of an auxetic material based on arranged cylinders/rods, schematically illustrated in Fig. 1. While touching, the rods may be encaged. Recently we developed a calculus for classification of configurations of infinite straight cylinders, by introducing so-called Chirality and Ring matrices, and invariants built on them [1, 2]. We verified our calculus considering touching cylinders. Starting from configurations of 7 mutually touching equal round cylinders (Fig. 2a) we constructed up to 10 mutually touching elliptical cylinders (Fig. 2b) and proved that this is the upper bound for mutual touching in 3D space [2]. We found that the entanglement of the cylinders may happen even when mutual touching is replaced by impenetrability and extended our calculus to deal with the entanglement of straight lines/rods.



**Figure 1.** A schematic for the "random" rods and a working multi-pod model with Poisson's ratio -1.

Here we suggest a possibility to create "random" entangled structures of rigid rods in an elastic matrix that would behave auxetically, well below the known mean-field lower limit of  $1/4$  for Poisson's ratio for rods in a dipole approximation. The elastic matrix would play a role of a support for embedded rods that is doomed to expand or shrink while the rods try to preserve their entanglement invariants, controlled by the chirality matrix [1, 2].



**Figure 2.** a) 7 mutually touching equal round cylinders; b) 10 mutually touching elliptic cylinders.

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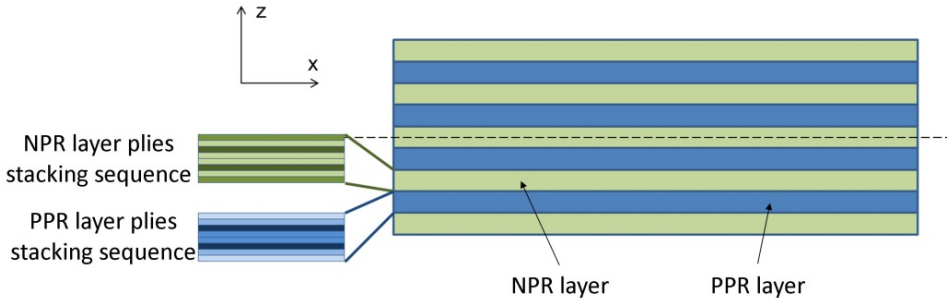
# Enhanced stiffness composite laminates through Poisson's ratio mis-match

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The possibility of enhancing the stiffness of layered composite systems through combining layers with mis-matched (positive and negative) Poisson's ratios has been suggested through modelling studies [1-4]. Recently, Classical Laminate Theory (CLT) was used to design hierarchical laminates comprising of layers, themselves comprised of several plies, of continuous fibre-reinforced matrix material with enhanced stiffness through Poisson's ratio mis-match of the layers [5] (Figure 1). In this paper, we report an experimental demonstration of the stiffening effect in carbon fibre-reinforced epoxy composite laminates.

Unidirectional composite specimens were first made from Toray T700S Fibre and TenCate E726 Epoxy pre-preg. The unidirectional composites were characterised for their mechanical properties, using a tensile testing machine combined with Digital Image Correlation (DIC), to provide the pre-preg input parameters for CLT design calculations. NPR layer and PPR layer symmetric laminate stacking sequences  $[60^\circ/15^\circ]_S$  and  $[\pm 30^\circ]_S$  were identified having the same Young's modulus but different (negative and positive, respectively) in-plane Poisson's ratios for loading along the  $x$  direction. Laminates comprising 12 plies in total were then made for each stacking sequence (so  $[60^\circ/15^\circ]_{3S}$  and  $[\pm 30^\circ]_{3S}$  for the NPR and PPR laminates, respectively), and for a hybrid laminate comprising of alternating 4-ply layers of each sequence ( $[60^\circ/15^\circ]_S, [\pm 30^\circ]_S, [60^\circ/15^\circ]_S$ ). Good agreement was found for the CLT predictions and experimentally measured values of  $E_x$  and  $\nu_{xy}$  (Table 1). A substantial (29%) increase in stiffness was achieved for the hybrid laminate over the laminates comprising of just one stacking sequence, providing experimental confirmation of the Poisson's ratio mis-match stiffening concept.



**Figure 1.** Hierarchical laminate composite comprising auxetic (NPR) and positive Poisson's ratio (PPR) layers, each comprising a sequence of plies.

**Table 1.** Predicted and measured laminate Young’s modulus and in-plane Poisson’s ratio values for tensile loading in the  $x$  direction.  $\langle E_x \rangle$  is the average of the  $E_x$  values for the NPR and PPR configurations.

Laminate id	Stacking sequence	Predicted $E_x/\langle E_x \rangle$	Predicted $\nu_{xy}$	Measured $E_x/\langle E_x \rangle$	Measured $\nu_{xy}$
NPR	$[60^\circ/15^\circ]_{3S}$	1.011	-0.137	$0.972 \pm 0.029$	$-0.210 \pm 0.050$
PPR	$[\pm 30^\circ]_{3S}$	0.989	1.336	$1.028 \pm 0.059$	$1.550 \pm 0.034$
Hierarchical NPR/PPR/ NPR	$[60^\circ/15^\circ]_S$ , $[\pm 30^\circ]_S$ , $[60^\circ/15^\circ]_S$	1.280	0.438	$1.293 \pm 0.023$	$0.429 \pm 0.024$

## Acknowledgements

This work was undertaken as part of a final year Bachelor of Engineering undergraduate project in the Department of Engineering and Mathematics at Sheffield Hallam University.

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# Numerical investigation of tubular structures generated by cutting method and pattern scale factor (PSF) method

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Auxetic materials and structures have attracted significant interest due to their uncommon mechanical behaviour. They will shrink (expand) laterally under compression (tension). Auxetic tubular structures have been used as oesophageal stents. Inspired by the recent kirigami method and the pattern scale factor (PSF) adjustment method, we designed several tubular structures. The tensile auxetic performance of these tubes was investigated using validated finite element analysis (FEA) to explore their properties. The results demonstrated that the random cut method was not suitable for designing auxetic tubular structures. Vertical and horizontal (V-H) cut approach was suitable, but the change of the tubular diameter was lower than the tubular structures generated by the PSF adjustment method.

# Chiral phonons and anomalous thermal expansion in $\text{BiB}_3\text{O}_6$

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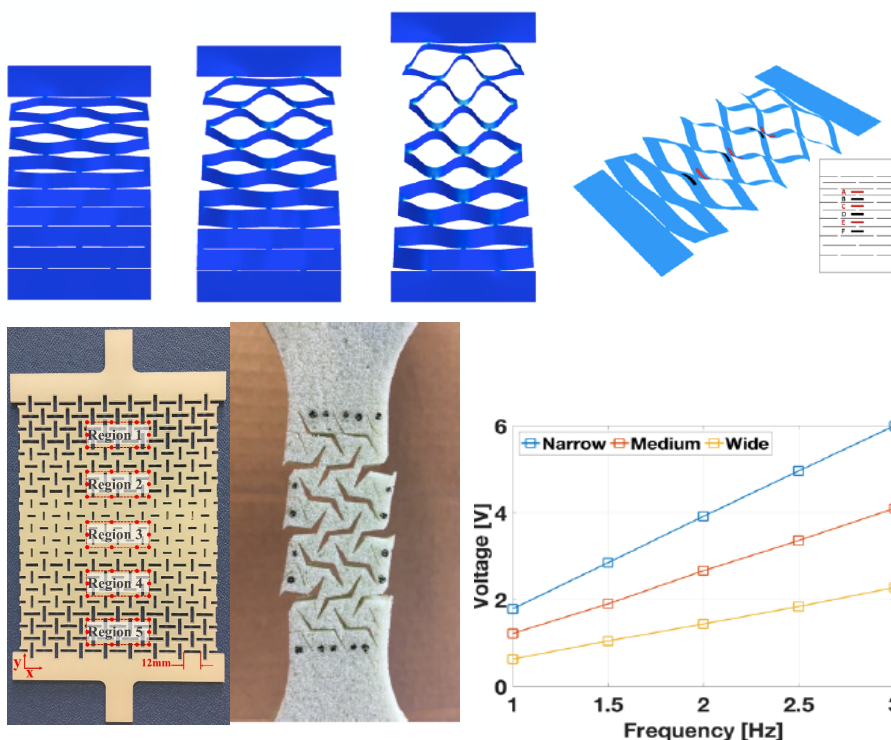
The vibrational origins of positive and negative thermal expansion have been studied in the chiral monoclinic solid  $\text{BiB}_3\text{O}_6$  using *ab initio* computational techniques. Librations of rigid borate units, elastic anisotropy, and chiral revolutions of bismuth atoms were all found to contribute to both positive and negative axial thermal expansion. The chirality of the lattice therefore contributes directly to anomalous thermal expansion by allowing the longitudinal acoustic branches to display opposing circular polarizations. Chirality therefore acts as a type of flexibility in this structure, giving freedom for certain types of motions which affect the properties of the bulk.

# Gradient and discontinuous architectures in Kirigami and tessellated perforations: mechanics and applications in flexible electronics, energy harvesters and foams

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We describe here the development of non-uniform gradient or tessellated architectures of cuts and perforations exhibiting unusual deformation mechanisms in substrates ranging from piezoelectric films to closed cell foams. The gradient and non-uniform architectures are created applying Kirigami (Origami and cuts) and machined perforations to obtain local stiffness and curvature patterns, large stretchability and voltage outputs combined with the use of topological electrodes for charge cancellations. We describe the applications of these architectures for wireless biomedical sensors, shape-change morphing structures and novel types of foams with auxetic deformation mechanisms.



# Finite element modelling of oblique impacts on auxetic structures for potential use in sports safety devices

T. Shepherd<sup>1</sup>, K. Winwood<sup>1</sup>, P. D. Venkatraman<sup>1</sup>,  
A. Alderson<sup>2</sup> and T. Allen<sup>1</sup>

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Auxetic materials and structures can demonstrate enhanced mechanical properties, such as increased resistance to indentation, increased energy absorption and synclastic curvature. These characteristics make auxetics candidates for enhancing sports safety devices. Previous work has validated finite element models of auxetic structures for normal impacts up to 5 J [1], and this work extends the validation to oblique impacts as these are relevant to sports safety devices, such as body padding, crash mats and helmets. Oblique impacts are an important consideration when investigating helmets, for example, as rotational acceleration is thought to be a main contributor to minor traumatic brain injuries (e.g. concussion), despite most helmet standards only considering linear acceleration [2]. Three anti-tetra chiral auxetic structures (with different overall designs) and a non-auxetic equivalent were modelled and finite element simulations were run at impact angles of 70° (relative to normal impacts) for impact energies up to 5 J. The structures were additively manufactured from a thermoplastic polyurethane (NinjaFlex®, NinjaTek), and impact tested using a bespoke instrumented drop tower coupled with a high-speed camera. Experimental results for peak force/acceleration, strain and impact time were compared to those from the finite element simulations and the findings will be presented in this presentation. The validated models can be used to further investigate the potential use of auxetic structures in sports safety devices, where structures could be tailored to limit acceleration under impact.

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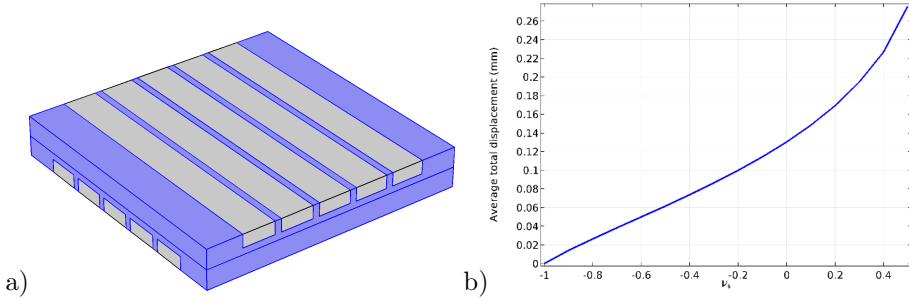
# Heat exchanger with auxetic material

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Materials with a negative Poisson's ratio (NPR) have been known for over 100 years. In the early 1900s, a German physicist Woldemar Voigt was the first who reported this property and his work suggested that the crystals can become thicker laterally when stretched longitudinally. Unfortunately, it was ignored for a few decades [1-4]. Simple mechanical and thermodynamical models, which show negative Poisson's ratio (auxetic behavior) were found in the 80s of the 20th century [1-4]. In 1981 Lorna Gibson [2] theoretically and experimentally analyzed the model of cellular material as a simple, two-dimensional array of hexagonal cells in order to identify and analyze the mechanisms by which it deforms. In 1987 materials with NPR are referred to us now as auxetics [5] and some researchers reviewed auxetics [e.g. 6]

In this research, the thermal properties of auxetic materials [7-9] are analyzed using the Finite Element Method [10]. Auxetics are applied as part of heat exchangers. The influence of Poisson's ratio of material used to build a thermally loaded structure of crossflow heat exchanger (see Figure 1a) is investigated. We can observe that displacement are smallest for auxetic material (see Figure 1b).



**Figure 1.** (a) View of cross-flow heat exchanger (gray - fluid channel and blue - auxetic) and (b) average total displacement of the heat exchanger as a function of Poisson's ratio of the material.

## Acknowledgements

This work has been supported by a grant from the Ministry of Science and Higher Education in Poland: 02/21/DSPB/3544/2019 and 02/21/SBAD/3558/2019. The simulations have been made at the Institute of Applied Mechanics, Poznan University of Technology (website: <http://am.put.poznan.pl/en/home/> ).

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# Odd elasticity

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The theory of elasticity provides a foundation for describing the mechanics of deformations of continuous media. However, elastic theories of active matter must confront a fundamental challenge: the starting point of elasticity, the elastic energy, is not well defined due to microscopic activity. We introduce Odd Elasticity as a generalized theory of continuum mechanics that breaks key symmetries of the elastic (stiffness) tensor otherwise required by conservation of energy. We show that odd elasticity describes solids in which activity depends on the deformation of microscopic bonds. As a minimal model that produces odd elasticity upon coarse graining, we consider active metamaterials in which internal torques are actuated in response to compression or extension of the beams. Our odd-elastic theory, corroborated by simulations, sheds light on a rich phenomenology, including activity-induced auxetic behavior, active elastic waves and instabilities. Our work revisits the foundations of continuum mechanics and provides a blueprint for the design of active elastic engines, which utilize a strain cycle to convert microscopic activity into useful mechanical work.

## Acknowledgements

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# Data based approach for analysing negative Poisson's ratio systems with different scales

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Negative Poisson's ratio (NPR) structures and materials have many unique properties and potential applications. Several mechanisms of Auxeticity has been discovered at different scales including macro, micro, nano and atomic levels, which influences the physical properties of the material in different ways. This paper report a recent work in analysing Auxetic behaviours through a data driven approach. A data system is used to develop structures with targeted Poisson's ratio. The system combined a python program for producing connected beams from randomly distributed point based on probability of dispersion number and divergence judgement. An interface is developed within the Abaqus kernel with automatic function of updating the key parameters following genetic algorithm. This program is used to automatically search or design new structures. The results shows that it is able to discover existing Auxetic structures and predict new structures. 3D printing of soft rubberlike plastic materials were produced and tested to validate the predictions. The data-led approach is also used in analysing directional Poisson's ratio of some lattice space groups through first-principles calculations. Through link with an open source molecular model database (Crystallography Open Database), a large number of compound molecular structure is established. Structural optimisation and elastic constant calculation is performed based on the density functional theory. The calculated elastic constants matrix is used to calculate the directional Poisson's ratio. Three-dimensional Poisson's ratio map of different lattice system were established. Some key results and detailed analysis of the new structures are presented. The potential link between simulations at different scales and modelling programs is discussed.



# Elastic properties of two-dimensional systems of hard cyclic tetramers

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Significant progress in nanoscience makes it possible to produce nanoparticles with the required geometry for assembling nanostructured materials [1]. This motivates studies of the role of particle geometry and its influence on various properties, including the elastic ones, of systems formed by them. In particular, it gives the possibility of creating auxetic materials at nanolength scales - nanoauxetics.

The present work focuses on elastic properties of systems composed of two-dimensional molecules, called planar hard cyclic tetramers. Each tetramer is composed of four hard discs (atoms) which centres form a square. The tetramer “molecules” can have various anisotropies described by the anisotropy parameter,  $\alpha$ , which is defined as the ratio of the square side and the disc diameter. It is known that even at  $\alpha = 1$  systems created by the tetramers present a rich phase diagram which has been studied using mechanical simulations [2]. The elastic properties of the tetramers have been evaluated by Monte Carlo (MC) simulations in the isobaric-isothermal ensemble [3,4]. In a work performed for  $\alpha = 1$ , it has been found that the Poisson’s ratio of the tetramer system is negative in main crystallographic directions [5]. In the present work, it has been shown that, depending on the anisotropy parameter, the tetramers form various phases which represent all the possible Bravais lattices in 2D space: oblique, rectangular, centered rectangular, hexagonal, and square. It was found that, depending on  $\alpha$ , the considered systems can show auxetic, partially auxetic, and non-auxetic behavior. The Poisson’s ratio observed in the studied systems varied from  $-0.59$  to  $0.77$ .

## Acknowledgements

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# Analysis of 3D metallic auxetic structures at high rates of strain using finite element DIC

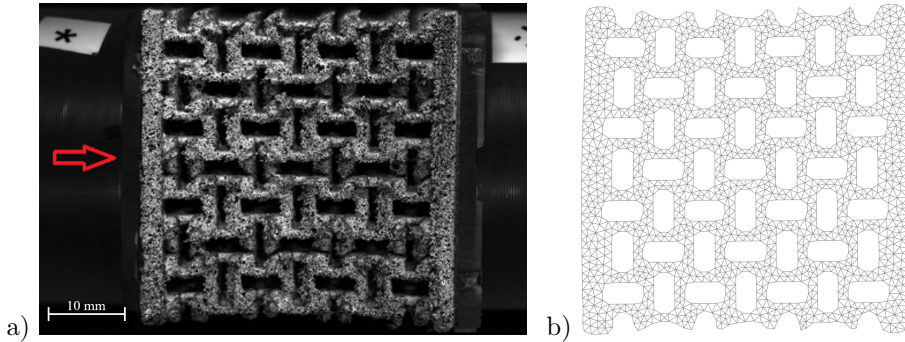
A. Trippel<sup>1</sup>, G. C. Ganzenmüller<sup>1,2</sup>, and S. Hiermaier<sup>1</sup>

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The structural response of auxetic 3D-printed metamaterials, i.e., structures with negative Poisson's ratio, is dependent on loading rate. At quasi-static conditions, auxetic structures generally exhibit well defined negative Poisson's ratio over a wide range of strains. However, at dynamic rates of strain, this is not necessarily the case: the magnitude of the rate of strain determines whether an auxetic effect occurs or the structure collapses. If the structure does not have enough time to achieve dynamic equilibrium, it experiences structural failure similar to pore collapse in foams, before auxetic behaviour can occur.

To provide an in-depth understanding of a structure and collect data in order to accurately model and simulate the metamaterial, a detailed analysis of the structural response is mandatory. The analysis is performed often using Digital Image Correlation (DIC). DIC is a popular method, which is easily commercially available. However, DIC applied to slender structures such as auxetic lattices often yields inaccurate measurements, because the displacement field is excessively smoothed in space. Therefore, typical commercial tools tend to reach their limits when it comes to its application on auxetic structures.

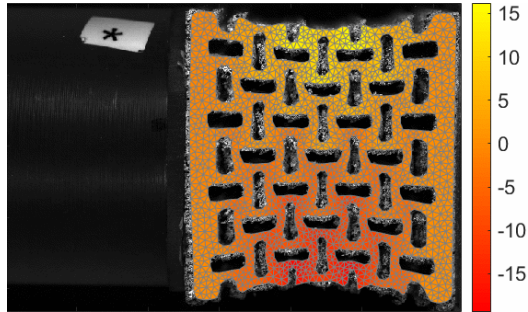


**Figure 1.** a) Recording of an auxetic structure in the DIHB, indicating the direction of the load, and b) its corresponding FE mesh for DIC evaluation focused only the lattice structure.

This work investigates an alternative approach for obtaining accurate deformation data for Auxetic structures under dynamic loading. To this end, we utilize

a Finite-Element based DIC procedure [1] and generate dynamic loading with a Direct Impact Hopkinson Bar (Fig. 1). This setup allows for obtaining precise force data at well-defined rates of strain, and accurate displacement fields, consistent with the true deformation of the lattice structure (Fig. 2).

Here, we apply this approach to a number of different 3D auxetic metal (SLM) specimens. We report their structural response, comparing quasi-static and dynamic rates of strain. Additionally, the work provides an insight in the application of a Finite Element based DIC and discusses the results.



**Figure 2.** The results of the last image recorded are shown, revealing the structural response. The colour indicates displacement in load direction in pixel. Strain rate: ca.  $250 \text{ s}^{-1}$ .

## Acknowledgements

I would like to express my very great appreciation to Francois Hild of LMT Cachan for his valuable help in applying the FE based DIC to our experiments. His willingness to give his time so generously has been very much appreciated

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# Extension of cylindrically anisotropic chiral tubes of the cubic crystals obtained by rolling up the crystal planes (110) and (111)

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We analyzed variability of Young's modulus and Poisson's ratios of cylindrically anisotropic chiral tubes obtained by rolling up the cubic crystal planes (110) and (111). It is assumed that crystallographic axis normal to (110) (or (111)) crystal plane coincide with radial axis of the tube. Two other axes are rotated on chiral angle  $\psi$  in plane of the plate so one of them coincide with longitudinal axis of the plate. The tube structure symmetry is reduced relative to symmetry of the cubic crystal due to influence of the chiral angle.

The tube symmetry corresponds to symmetry of monoclinic crystal with 13 compliance coefficients in the case of rolling up (110) crystal plane, and in the case of rolling up (111) plane – triclinic (21 coefficients). With use of known solution of problem of cylindrically anisotropic tube extension with the most general anisotropy, expressions of Young's modulus and Poisson's ratios, which characterizes deformation in radial and angular directions, dependencies on compliance coefficients of cubic crystal, ratio of tubes radii and chiral angle were obtained. Variability analysis of these characteristics were performed and results were compared with results obtained for tubes rolled up from (001) plane [1]. The dependencies of Young's modulus and Poisson's ratios of tubes obtained by rolling up the crystals planes (111) and (110) are periodic functions of chiral angle with period  $\pi$ . Surfaces of this characteristics are symmetric respective  $\pi/2$ . Topology of Young's modulus and Poisson's ratio surfaces are much more complex for the tubes rolled from the crystal planes (110) and (111) than for the tubes rolled from (001) crystal planes. This surfaces have much more complex parametric dependencies on main determining parameters.

At zero chiral angle there is no difference between the behavior of tubes obtained by rolling up the crystal plates (110) and (001). At this chiral angle there are 150 auxetic tubes rolled up from (111) plane and 20 auxetic tubes from (110) plane. When the chiral angle takes on a value of  $\pi/2$  there are 8 (111) auxetic tubes and more than 600 auxetic obtained by rolling up (110) crystal plate. When the chiral angle changes in the range from 0 to  $\pi/2$  and the ratio of the tube radii changes in the range from 1.01 to 10 the number of auxetic tubes are about 850 and 700 in the case of rolling up (110) and (111) crystal planes, respectively. Auxeticity in radial direction of tubes obtained by rolling up (110) crystal planes significantly increases compared with tubes rolled up from (111) or (001) planes.

Chirality angle and crystal plane choice for tube rolling up is affect significantly on auxetic behavior of tube. The number of auxetics and magnitude of negative Poisson's ratio changes greatly for tubes rolled up from (110) and (111) crystal planes at different chirality angles.

## Acknowledgements

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# Design of materials with enhanced mechanical properties

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The increased fabrication accessibility, such as additive manufacturing, brings tremendous interest in designing novel materials with enhanced properties, such as auxetic materials and materials with enhanced buckling strength. Auxetic materials are of great interest for a wide range of applications due to their enhanced mechanical properties, e.g., shear or indentation resistance and extraordinary damping properties [1,2]. Various linear auxetic materials have been created and fabricated considering small deformations. However, experiments have shown that auxetic materials are highly sensitive to deformations and that auxetic properties vanish at finite strains [2], except for buckling-induced auxetic materials that have been obtained via pattern transformations to retain auxetic properties at finite strains [3]. In addition to auxetic behavior, material buckling strength has been of great importance and critical to the exploitation of materials. Previous studies have investigated a wide range of material configurations in search for improved buckling strength and discovered that geometric attributes play an essential role [4].

In the field of material design, topology optimization methods have been successfully applied to design materials with exotic properties via redistributing base material in the periodic unit cell [5,6]. Auxetic materials with programmable Poisson's ratio under finite deformations have been obtained in [5]. Novel first-order hierarchical type materials with enhanced buckling strength have been designed for hydrostatic and uniaxial compression [6], where both long- and short-wavelength buckling has been considered in the optimization procedure based on homogenization theory, a linearized stability criterion and Bloch–Floquet theory.

This study explores material designs with enhanced properties, including auxetic behavior at finite strains and buckling strength, via topology optimization methods. First, the design approach proposed in [5] is employed to further explore different 3D auxetic material architectures with programmable Poisson's ratios under finite deformations. Several auxetic material configurations are obtained by changing symmetry on the unit cell. The optimized material configurations are further parameterized concerning Poisson's ratios in sequential shape optimization. A class of auxetic material configurations can be directly obtained using the parameterized architectures for any prescribed negative Poisson's ratio, and the Poisson's ratio is independent of deformations over a large strain range. Second, systematic material designs are discussed to enhance material buckling strength based on the study in [6].

## Acknowledgements

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# Crushing analysis and collaborative optimization design for a novel crash-box with re-entrant auxetic core

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Crash-box is a significant part of automotive passive safety system and serves as an impact energy absorption device in frontal impact scenario. This paper explores a novel crash-box by integrating an outer thin-walled tube and an inner auxetic cellular core. Numerical simulations show that introduction of the auxetic core enables the novel crash-box simultaneously possess the capacities of structural crashworthiness and occupant protection. The effects of independent geometric parameters on crash-box capacities are studied. To improve the capacities of crash-box under low-speed (15km/h) and high-speed impact cases, collaborative optimization has been performed based on the least square support vector regression (LS-SVR) method and an improved multi-objective particle swarm optimization (MOPSO) algorithm. The optimal design of the novel crash-box shows to achieve 15% reduction in the peak impact force (PIF) and 15% increase in the mean impact force (MIF) under low-speed impact, and 15% increase in the specific energy absorption (SEA) under high-speed impact. The proposed crash-box and its collaborative optimization design method provide extensive references for the application of auxetic structure in vehicle engineering domain.



# Applications of auxetic structures in automobile

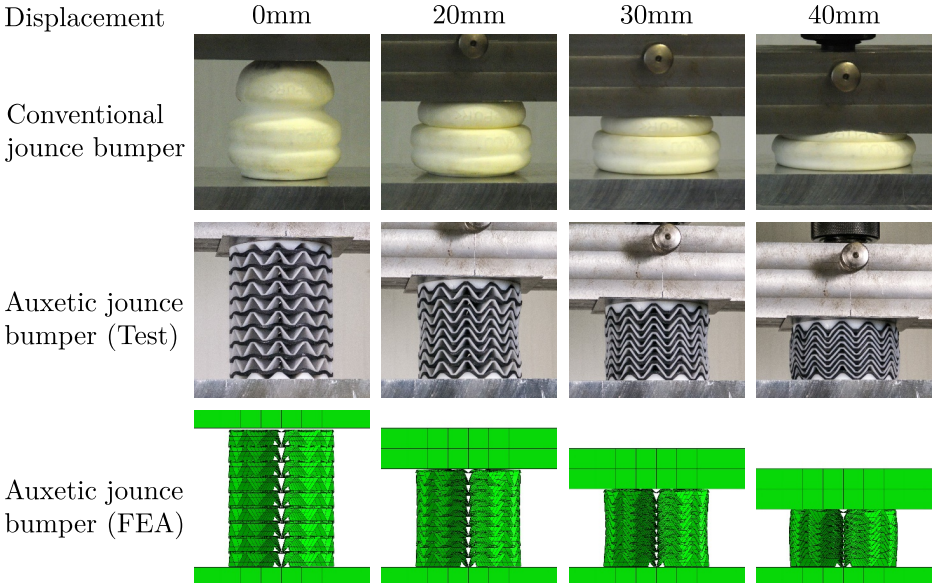
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Double-V auxetic structure have great energy absorption energy through specific structural and base material design. It can be applied in some automotive components, including bumper, bushing, crash box and other important components. Since the load-displacement curve of conventional jounce bumper sometimes cannot reach ideal zone result from the limitation of its structure. A novel auxetic jounce bumper was proposed based on the 2D Double-V auxetic structure in this paper. A parametric modelling and analysis method were proposed. The mechanical performances of conventional jounce bumper and auxetic jounce bumper were compared using numerical and experimental methods. Compared with conventional jounce bumper, the load-displacement curve of auxetic jounce bumper had linearer stiffness at small displacement and smoother transition area at moderate displacement. Then the influences of structure parameters on the mechanical performance were also researched. Suspension and vehicle virtual prototypes were employed to evaluated jounce bumpers, and the auxetic jounce bumpers were optimized where maximum acceleration of driving through bump was minimized. In addition, we also developed auxetic tire, which will be discussed in this paper.

**Table 1.** Deformation shapes of conventional and auxetic suspension jounce bumper.



# Chiral mechanical metamaterials

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After a brief introduction into 3D metamaterials in general [1] and into effective-medium descriptions of chiral mechanical continua in particular [2], I will focus on our recent results on the static and the dynamic properties of 3D chiral mechanical metamaterials – both, in experiment and in theory.

Concerning the static case, I will start by briefly recalling our previously published work [3] on push-to-twist conversion in 3D chiral cubic microstructured polymer-based mechanical metamaterials manufactured by 3D laser lithography. These twist effects are forbidden in Cauchy elasticity. Lately, it has become clear to us that not only Eringen micropolar elasticity can describe these effects [3], but also Willis elasticity [4]. Under our conditions, Willis elasticity has only one additional parameter with respect to Cauchy elasticity [4]. In addition, I will discuss our work on tailoring the corresponding characteristic length scale such that large twist effects survive up to total numbers of 3D metamaterial unit cells exceeding one hundred thousand [5].

Concerning the dynamic case, we have recently observed the phenomenon of "acoustical activity" (or "mechanical activity"), the mechanical counterpart of optical activity, which is a paradigm of chirality [6]. We have achieved and characterized experimentally linear polarization rotations as large as 22 degrees per unit cell [6]. Here, the metamaterial design closely follows that presented in [3]. Possibly, I will also present results based on a rather different chiral 3D unit cell [7]. This design leads to yet larger measured polarization rotation angles [7]. Furthermore, I will discuss our designs of 1D chains of alternating 3D chiral unit cells exhibiting topological 1D band gaps connected to topologically protected twist edge states. A micro-mirror at this edge can be applied in the sense of a scalable resonant mechanical laser beam scanner [8].

## Acknowledgements

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# Controlling the negative thermal expansion of ReO<sub>3</sub>-type fluorides by the deliberate introduction of excess fluoride

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Several cubic ReO<sub>3</sub>-type fluorides, such as ScF<sub>3</sub> [1] and CaZrF<sub>6</sub> [2], have been shown to display strong negative thermal expansion over a wide temperature range. They combine negative thermal expansion with low absorption from the mid-IR out into the UV, and processability as ceramics, suggesting application in controlled thermal expansion optics. However, they are susceptible to undesirable phase transitions on exposure to modest stress and efforts to tune their thermal expansion by simple solid solution formation tends to exacerbate this problem. The deliberate introduction of interstitial fluoride, by going off stoichiometry from that of the ideal ReO<sub>3</sub>-composition, provides a method of tuning thermal expansion while improving the resistance of the material to unwanted pressure/stress induced phase transitions. This will be illustrated with reference to YbZrF<sub>7</sub> [3] and the excess fluoride solid solution system Mg<sub>1-x</sub>Zr<sub>1+x</sub>F<sub>6+2x</sub> [4]. In these systems the incorporation of interstitial fluoride changes the framework connectivity and hence the response to both temperature and pressure. However, in some other systems the incorporation mechanism is different and it does not provide for effective control of thermal expansion.

## Acknowledgements

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# From nano- to macro-auxetics: a simple three-parameter model of macroscopic auxetic structure inspired by penta-graphene

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Penta-graphene (PG) is a new carbon allotrope which has been proposed theoretically based on *ab initio* calculations [1]. The structure of PG resembles the well-known Cairo tiling, consisting solely of pentagons, which in PG are formed by carbon atoms connected with strong covalent bonds, both of the  $sp^2$ - and  $sp^3$ -type.

Since its discovery, PG has attracted much interest, mostly because of its unique electrical, optical and chemical properties. However, PG also possesses interesting mechanical properties, including but not limited to very high in-plane stiffness, comparable to that of graphene. PG is also predicted to be characterized by a negative Poisson's ratio [1–4]. Therefore, it belongs to a class of metamaterials called auxetics, which – due to their very unusual mechanical behavior and many possible practical applications – attract more and more attention nowadays.

Recent calculations [4] have shown that PG can be considered as a completely auxetic structure, as its Poisson's ratio (PR) is negative for all deformation directions lying in the plane of its structure. This feature is very rare, as most of the auxetic crystals display auxeticity only for some particular crystallographic directions. In [4] it has been also reported that the PR of PG decreases with the increasing strain, remaining negative even at very high strains. While both of the above-mentioned features make PG a particularly interesting metamaterial, its current practical applications are completely limited by the fact that it has not been synthesized yet. However, an attempt to transfer the mechanism of PG auxeticity into the macro-scale – and to build a macroscopic mechanical structure inspired by PG – can be made.

The presentation will aim to answer the question whether it is possible to produce a macroscopic equivalent of PG: a mechanical structure with a similar (*i.e.* pentagonal) topology and similar (*i.e.* auxetic) mechanical properties. For this purpose, a simple three-parameter model was proposed, within which the structure of PG was modeled as a network of nodes (corresponding to carbon atoms) connected with harmonic springs (corresponding to carbon-carbon bonds). The angular contributions (which capture energy changes originating from bending of bonds) were also included in the adopted model and also described using a harmonic potential. These contributions were found in [4] as essential for the auxeticity of PG.

Using the proposed model it was studied how its mechanical properties depended on its three parameters: two parameters defining the structure and one parameter describing the interactions. For this purpose, the elastic constants and the mechanical moduli were calculated using the molecular statics method. The relation between the parameters of the model and its mechanical properties was characterized quantitatively and the region of auxeticity (for which  $PR < 0$ ) was determined. The results have shown that – despite its significant formal simplicity – the considered structure may display a complete range of mechanical behaviors, being even perfectly auxetic (with  $PR = -1$ ) or perfectly incompressible (with  $PR = 0.5$ ).

Although the proposed model is a considerable simplification of reality (the linear mechanical behavior of the model constituents is assumed) the obtained results strongly suggest that it should be possible to create a macroscopic equivalent of PG, which is also auxetic. The possibilities of manufacturing the proposed structure (*e.g.* using the 3D printing technology) will be also discussed during the presentation.

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# Simple models with unusual properties

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Systems with Poisson's ratio [1] reaching negative values [2-5] are called auxetics [6]. Some simple models, studied by analytic methods and computer simulations, will be reviewed in this context and a few mechanisms leading to auxeticity will be discussed [7]. During the lecture it will be also explained why auxetics are better than miotics [7].

## Acknowledgements

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# Towards determination of elastic properties of liquid crystal blue phases

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Blue phases (BPs) are highly self-assembled three-dimensional mesoscopic structures which typically occur between the low-temperature cholesteric (chiral nematic) phase and the high temperature isotropic (liquid) phase. They are unique types of liquid crystal which form structures with crystal symmetry (the body centered cubic and simple cubic). Previously BPs were found to be stable only over a very narrow temperature range, but more recently they have been stabilized over considerably larger temperature ranges. Stabilizing the BPs has opened up a new era for blue phase research, with possible applications in next-generation displays and photonics. There is evidence that in modification of key features of BP an important role play elastic properties. In particular a lowering of operating switching voltage can be realized via changing the Kerr constant which depends inter alia on the elasticity of BPs. Unfortunately, BP samples are polycrystalline and represent an extremely soft material what makes the estimation of the single crystal elastic constants very difficult in practice.

In this presentation we consider the modified Gerber model which in its original form relates the Kerr constant to the birefringence, dielectric anisotropy, pitch length and the average elastic constant of the chiral liquid crystal. The values of the corresponding parameters (particularly elastic part) are however mostly unknown for BPs and the data obtained with a low temperature cholesteric phase are used and commonly directly applied to the BPs. In the modified model the Kerr constant and the parameters obtained for the BPs are exploited to test a role of effective birefringence and lattice spacing. This approach makes feasible the estimation of the effective contribution of the elastic part of BP samples.

## Acknowledgements

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# Enhanced hexa-missing rib auxetics with tunable isotropic negative Poisson's ratios for large deformations

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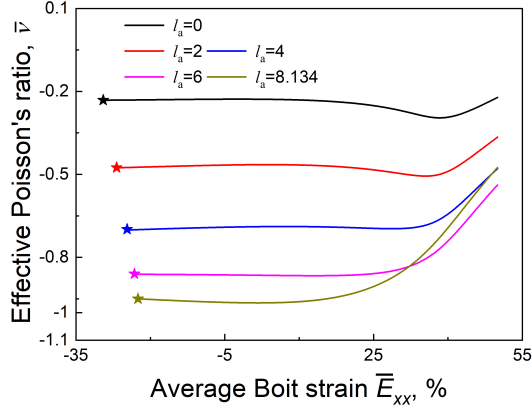
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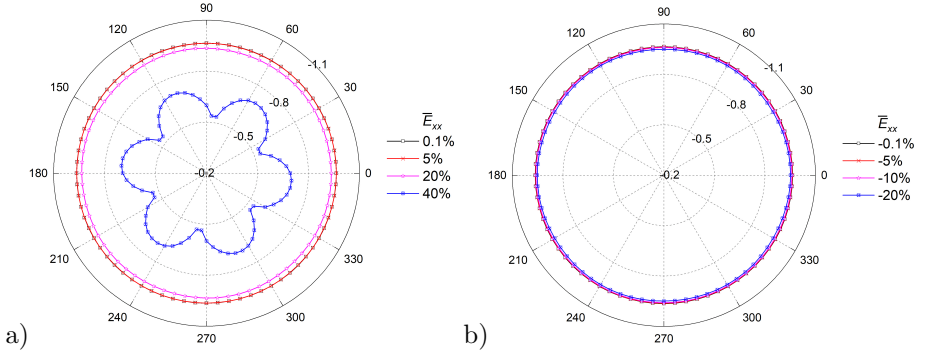
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Standard hexa-missing rib structure (i.e., missing rib structure with six zigzag ligaments) is a typical initially in-plane isotropic auxetic structure and performs relatively constant Negative Poisson's ratio (NPR) in a large strain range. However, its auxeticity is relatively weak and the isotropy is degraded rapidly in large deformation. The present work aims to improve these two mechanical properties, without significantly compromising the constant NPR performance in the regime with geometrical nonlinearity effect. By analyzing the elastic deformation profile of a standard hexa-missing rib structure, it is revealed that its weak auxeticity and rapidly losing isotropy are owing to the lack of structural supports between the ligaments. To facilitate the development of this deformation mechanism, an enhanced design with honeycomb reinforcement is proposed subsequently. The proposed enhanced hexa-missing rib structure presents improving auxeticity and isotropy properties with the increment of edge length of the reinforced honeycomb, and largely maintains the approximately constant NPR performance at the meantime. Particularly, a Poisson's ratio close to -1 is obtained when the reinforced honeycomb is inscribed in the zigzag ligaments. It is further revealed that to render the bending ligaments more flexible will help to maintain the constant NPR limit. Based on the former proposed design, a new design with wavy bending ligaments is hence presented.



**Figure 1.** Effective Poisson's ratio evolutions of the enhanced hexa-missing rib structures with different reinforced honeycomb edge length  $l_a$ . The colored pentagram represents the FE calculation fails due to contact.



**Figure 2.** a) Tensile and b) compressive polar plots of effective Poisson's ratio for the enhanced hexa-missing rib structure with inscribed reinforced honeycomb ( $l_a = 8.134$ ) at different deformation level.

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