

7th International Conference

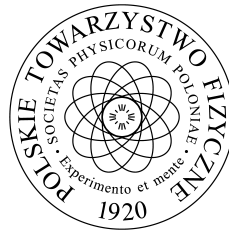
**Auxetics and other materials and models
with "negative" characteristics**

12th International Workshop

Auxetics and related systems

12–16 September 2016

Szymbark, Poland



ABSTRACT BOOK

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Auxetics and other materials and models with "negative" characteristics
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J. W. Narojczyk, J. Rybicki, and K. W. Wojciechowski

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Programme of the Meeting

| Monday 12.09.2016 | Tuesday 13.09.2016 | Wednesday 14.09.2016 | Thursday 15.09.2016 | Friday 16.09.2016 |
|----------------------------------|------------------------------|-----------------------------|---|-----------------------------|
| | 9.00 - 10.45 SESSION I | 9.00 - 10.45 SESSION I | 9.00 - 10.45 SESSION I | 9.00 - 10.45 SESSION I |
| | Coffe break | | | |
| | 11.15 - 13.00 SESSION II | 11.15 - 13.00 SESSION II | 11.15 - 13.00 SESSION II | 11.15 - 13.00 SESSION II |
| 13.00 - 18.00 | 13.00 - 14.30 Lunch | | | |
| Registration | 14.30 - 16.15 SESSION III | 14.30 - 19.00 Excursion | 14.30 - 15.40 SESSION III | |
| | Coffe break | | 15.40 - 17.00 Round table discussion | |
| | 16.45 - 19.00 | | 15.40 - 17.00 Poster Session and Young Researchers Forum | |
| 18.00 - 19.00 OPENING SESSION | SESSION IV | | | |
| 19.00 - Welcome Party | 19.00 - 20.00 Dinner | 19.00 - Banquet | 19.00 - 20.00 Dinner | |

CONTENTS

| | |
|--|----|
| <u>A. Airoidi</u> , A. Gilardelli, P. Panichelli, P. Astori, and R. Farinelli <i>Development and applications of composite chiral networks with auxetic behaviour</i> | 11 |
| <u>M. Bilski</u> and K. W. Wojciechowski <i>Equation of state and phase diagram of hard cyclic hexamers with various molecular anisotropy</i> | 13 |
| <u>R. Caruana-Gauci</u> , D. Attard, and J. N. Grima <i>A general wine-rack like model exhibiting negative Poisson's ratios and negative linear compressibility</i> | 15 |
| H. C. Cheng and <u>F. Scarpa</u> <i>Nonlinear bending and shear of composite sandwich beams with auxetic foam cores</i> | 16 |
| <u>S. Czarnecki</u> and T. Lewiński <i>Pareto optimal design of non-homogeneous isotropic materials properties for the multiple loading conditions</i> | 17 |
| <u>Y. Dobah</u> , M. K. B. To, F. Scarpa, and J. N. Grima <i>Auxetic dome-shaped cellular structures</i> | 18 |
| <u>M. R. Dudek</u> , R. Caruana-Gauci, K. K. Dudek, J. N. Grima, R. Gatt, K. W. Wojciechowski, and W. Wolak <i>Shape memory in magneto-auxetic systems</i> | 19 |
| <u>K. K. Dudek</u> , R. Gatt, L. Mizzi, M. R. Dudek, D. Attard, K. E. Evans, and J. N. Grima <i>Hierarchical systems with tunable mechanical properties</i> | 20 |
| <u>A. V. Dyskin</u> and E. Pasternak <i>Stability of extreme auxetic and incompressible elastic materials</i> | 21 |

| | |
|---|----|
| <u>R. Gatt</u> , K. M. Azzopardi, J. P. Brincat, M. R. Dudek, K. K. Dudek, and J. N. Grima <i>On the thermo-mechanical properties of layered crystals</i> | 22 |
| R. V. Goldstein, V. A. Gorodtsov, <u>D. S. Lisovenko</u> , and M. A. Volkov <i>The two-layer tubes-auxetics of cubic crystals</i> | 23 |
| J. N. Grima, R. Caruana-Gauci, E. P. Degabriele, K. K. Dudek, M. C. Grech, R. Gatt, L. Mizzi, and D. Attard <i>Some recent advances in negative materials and structures</i> | 24 |
| E. Harkati, <u>C. Abaidia</u> , A. Bezazi, N. Daoudi, and F. Scarpa <i>The effect of the density and the curvature of the walls on the elastic moduli of a new auxetic cell structure by a refined model</i> | 25 |
| D. M. Heyes, D. Dini, and A. C. Brańka <i>Nanowire stretching by Non-equilibrium Molecular Dynamics</i> | 27 |
| D. T. Ho and <u>S. Y. Kim</u> <i>Auxeticity due to elastic instabilities</i> | 28 |
| <u>H. Hu</u> and W. S. Ng <i>Deformation behavior of auxetic quadruple helix yarns under tension</i> | 29 |
| K. Hyżorek, P. M. Pigłowski, K. V. Tretiakov, and K. W. Wojciechowski <i>Elastic properties of Yukawa systems with nanochannels</i> | 32 |
| K. Hyżorek and K. V. Tretiakov <i>The molecular dynamics methods to study the confined system: thermal conductivity of liquid argon in nano-channels</i> | 33 |
| <u>H. Jopek</u> and T. Stręk <i>Computational modeling of thermoauxetic composite structures</i> | 34 |
| <u>C. Kern</u> , M. Kadic, and M. Wegener <i>Sign reversal of the Hall coefficient in three-dimensional metamaterials</i> . . | 35 |
| S. D. Li, K. Al-Badani, Y. Gu, M. Lake, and <u>J. Ren</u> <i>The effects of Poisson's ratio on the mechanical behaviour of embedded system in an elastic Matrix</i> | 36 |
| <u>T. C. Lim</u> <i>An auxetic structure with NTE characteristic</i> | 37 |

| | |
|--|----|
| <u>D. S. Lisovenko</u> , V. A. Gorodtsov, and R. V. Goldstein <i>Tension and torsion nanomicrotubes with cubic cylindrical anisotropy</i> . . . | 38 |
| S. Maćkowiak, D. M. Heyes, D. Dini, and <u>A. C. Brańka</u> <i>Friction of confined particle films under external load and shear by Non-equilibrium Molecular Dynamics</i> | 39 |
| S. Maćkowiak, S. Pieprzyk, D. M. Heyes, D. Dini, and A. C. Brańka <i>Non-equilibrium phase behavior of confined molecular films in low-speed regime</i> | 40 |
| <u>S. Mandhani</u> , P. Zolgharnein, A. Alderson, and I. ur Rehman <i>Tri-layered auxetic scaffold for bone regeneration</i> | 42 |
| <u>B. T. Maruszewski</u> and P. Fritzkowski <i>Effective Young's modulus and Poisson's ratio of the thermoelastic normal and auxetic plate determined from the extended thermodynamical model</i> . . | 43 |
| <u>P. H. Mott</u> , J. H. Roh, and C. M. Roland <i>Failure of classical elasticity in auxetic foams</i> | 44 |
| J. W. Narojczyk, M. Kowalik, and K. W. Wojciechowski <i>Poisson's ratio of the DC phase of hard dimers with arrays of nanochannels</i> | 45 |
| <u>N. Novak</u> , M. Vesenjak, and Z. Ren <i>Computational modeling of auxetic structures</i> | 46 |
| <u>E. Pasternak</u> and A. V. Dyskin <i>Wave propagation in materials with negative moduli</i> | 47 |
| P. M. Piękowski, K. V. Tretiakov, J. W. Narojczyk, and K. W. Wojciechowski <i>Elastic properties of mono- and polydisperse of Hard-Core Repulsive Yukawa Particles</i> | 48 |
| F. Porzio, É. Cuierrier, C. Wespiser, R. S. Underhill, and <u>A. Soldera</u> <i>Molecular simulation as a guide for potential auxetic materials</i> | 50 |
| <u>A. A. Poźniak</u> and K. W. Wojciechowski <i>Isotropic and continuous planar auxetics from hard star-shaped inclusions – numerics and experiment</i> | 51 |
| J. Qu, <u>C. Kern</u> , M. Kadic, and M. Wegener <i>Sign reversal of the thermal expansion coefficient in metamaterials fabricated via three-dimensional dip-in direct laser writing</i> | 53 |

| | |
|---|----|
| J. Roe, O. Duncan, T. Allen, L. Foster, P. Godbole, N. Jordan-Mahy, C. L. Le Maitre, and <u>A. Alderson</u> <i>The application of auxetic materials in tissue engineering</i> | 54 |
| <u>J. Rushchitsky</u> <i>Nonlinearity of elastic deformation and moderateness of strains as a factor explaining the auxeticity of material</i> | 57 |
| I. Shufrin, E. Pasternak, and <u>A. V. Dyskin</u> <i>The effective coefficient of thermal expansion of material with auxetic inclu- sions</i> | 60 |
| <u>T. Stręk</u> <i>Vibration properties of sandwich panel with folded plates core</i> | 61 |
| <u>K. V. Tretyakov</u> , P. M. Pięłowski, and K. W. Wojciechowski <i>Auxeticity of the Yukawa crystals with nanoslits and nonochannels</i> | 64 |
| P. Verma, M. L. Shofner, and <u>A. C. Griffin</u> <i>Reversibility of thickness change in nonwovens</i> | 65 |
| <u>R. I. Walton</u> <i>Anisotropic expansivity of flexible metal organic frameworks</i> | 66 |
| Y. C. Wang, M. W. Shen, and S. M. Liao <i>Microstructural effects on the Poisson's ratio and damping of discs</i> | 68 |
| <u>A. P. Wilkinson</u> <i>Negative thermal expansion and other anomalous properties in metal fluo- rides with structures related to that of ReO_3</i> | 70 |
| <u>S. Winczewski</u> , M. Y. Shaheen, and J. Rybicki <i>Structural and mechanical properties of pentagraphene: preliminary molecular statics/molecular dynamics studies</i> | 71 |
| <u>K. W. Wojciechowski</u> <i>Simple models exhibiting negative Poisson's ratio</i> | 72 |
| <u>W. Wolak</u> and M. R. Dudek <i>Auxeticity in a system of densely packed polymers</i> | 74 |
| P. Zolgharnein, A. Alderson, and I. ur Rehman <i>Piezo-morphic bone scaffold with auxetic behavior</i> | 75 |

Development and applications of composite chiral networks with auxetic behaviour

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Many studies have been conducted on the auxetic response of chiral topologies and some authors proposed the adoption of chiral networks for the development of morphing aerodynamic surfaces, capable of progressive shape variations [1,2]. A technological process was devised in [2] and improved in [3] to manufacture chiral networks made of thin composite laminates (Fig. 1), which were applied to develop an innovative aerodynamic profile that change its camber under the action of the aerodynamic force [4]. Moving from such results, further applications of chiral composite networks are presented in this work, referred to actuated morphing structures. The design of a morphing aileron is presented, with a chiral internal structure and diffused shape memory alloys actuators. The design process of the system involved an optimization process, performed on a condensed aeroelastic model, and a final assessment of a virtual prototype (Fig. 2). In a second application, the chiral configurations that can be obtained by applying the most recent version of the technological process are adopted to design a morphing high lift device with severe structural requirements. A combined actuation system is selected to maximize morphing capabilities, based on shape memory alloy actuators embedded in the skin of the airfoil and on rotative actuators acting on the nodes of the chiral internal structure. Finally, preliminary studies on the development of energy absorption systems based on thin chiral networks are presented.

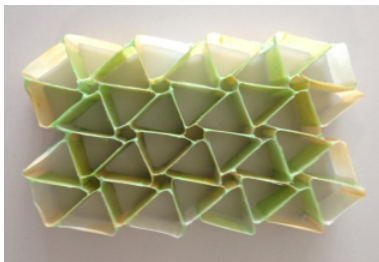


Figure 1. Composite chiral network.

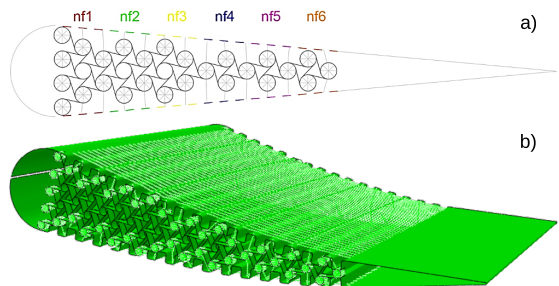


Figure 2. Actuated morphing aileron: scheme for condensed model (a) virtual assessment on complete model (b).

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Equation of state and phase diagram of hard cyclic hexamers with various molecular anisotropy

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Hard-body interactions, infinite at overlap and zero otherwise, constitute one of the simplest models describing various physical systems. Structures made of hard particles can play a role of purely geometric models of solids and can be very useful in study of impact of shape of molecules on their properties.

Two-dimensional hard cyclic hexamers (HCH) are constructed of six identical hard discs each, which centres form a perfect hexagon of the side σ , further taken as the unit of length. The ratio $d' = d/\sigma$, where d stands for the disc diameter, determines the parameter of molecular anisotropy (or roughness parameter) of such particles. Systems of HCH molecules of $d' = 1$ were studied previously [1-2] and they have been shown to form elastically isotropic phases, out of which the densest is chiral and exhibits negative Poisson's ratio [3-5]. Such value of Poisson's ratio leads to anomalous elastic properties of the materials [6, 7], which are presently known as auxetics [8-10], and which are currently experiencing increased interest [11-26] due to variety of potential applications. In the present work computer simulations are used to determine the phase diagram and equation of state of studied HCH systems for $d' \in (0.5, \infty)$. In order to locate the first-order phase transitions numerical determination of the free energies of the phases is made.

Acknowledgments

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A general wine-rack like model exhibiting negative Poisson's ratios and negative linear compressibility

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Negative linear compressibility (NLC) is the anomalous property of expanding in one direction when a compressive hydrostatic pressure is applied. One of the renowned mechanisms to exhibit this property is the wine-rack like motif deforming through hinging [1-3]. This motif is typically studied with all sides being equal in length. In this paper we consider a more general wine-rack like motif where only the opposite pair of sides are of equal length. The basic unit of such a general structure is not necessarily rhombic or rectangular but can be parallelogrammic.

This paper presents a discussion on the various anomalous mechanical properties exhibited by such a general wine-rack like motif. It is shown that this general structure could exhibit negative Poisson's ratios and negative linear compressibility both on-axis and off-axis. By means of an analytical model, this paper elucidates the various conditions necessary for such properties to occur. This model shows that the general wine-rack like motif could attain a wider spectrum of compressibilities compared to the simpler wine-rack like motif and at the same time potentially be able to explain the occurrence of NLC in more materials and structures.

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Nonlinear bending and shear of composite sandwich beams with auxetic foam cores

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In this work we present the manufacturing and testing of composite sandwich beams with carbon fibre prepregs skins and open cell PU foams with conventional (PPR) and auxetic (NPR) characteristics. We consider in particular the difference in flexural stiffness, shear and energy absorption between the different types of foam cores by comparing three types of sandwich beams, auxetic, conventional thin (same thickness of the auxetic) and conventional thick (same weight of the auxetic). The tests are carried out under 3-points and 4-points cyclic and direct loading tests. While the auxetic sandwich beams show slightly lower loss factors than those exhibited by the conventional sandwich beams under the same thickness, the loss value is however increased in the NPR case for large deformations. The shear modulus of the auxetic foam is lower than the one of the conventional foam material, although the density is higher. Zero-stiffness and negative stiffness effects are observed and discussed.

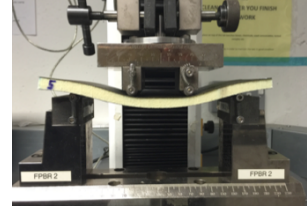


Figure 1. 4-point bending of a sandwich beam with auxetic core.

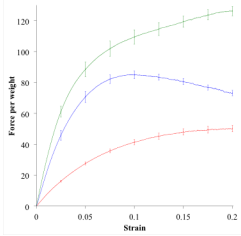


Figure 2. Specific force vs. strain for the sandwich beams under 4-point loading. Red: auxetic; blue: conventional (same thickness as auxetic); Green: conventional (same weight as auxetic).

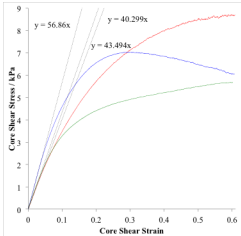


Figure 3. Core shear stress vs. shear strain for the sandwich beams under 4-point loading. Red: auxetic; blue: conventional (same thickness as auxetic); Green: conventional (same weight as auxetic).

Pareto optimal design of non-homogeneous isotropic materials properties for the multiple loading conditions

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The paper deals with finding efficient points (Pareto front) representing images $\wp^* = (\wp_1(C^*), \wp_2(C^*), \dots, \wp_n(C^*)) \in \mathbb{R}^n$ of the compliances $\wp_i(C^*)$, $i = 1, 2, \dots, n$ corresponding to n independent loading conditions along with the Pareto optimal points C^* denoting the non-homogeneous, isotropic Hooke elasticity tensors characterized by negative values of Poisson's ratio. The unit cost of the design is assumed as equal to the trace of the elastic moduli tensor C .

In the paper the weighted sum approach, as one of the most common transformation of the vector optimization problem into scalar valued optimization problem, is adopted. The merit function assumed: $\wp(C) = \eta_1 \wp_1(C) + \eta_2 \wp_2(C) + \dots + \eta_n \wp_n(C)$, $\eta_1 + \dots + \eta_n = 1$, $\eta_i \geq 0$, $i = 1, 2, \dots, n$ represents the weighted sum of the compliances corresponding to subsequent load conditions. The numerical results obtained show that the Poisson ratio being negative have a strong impact on Pareto optimal distribution of the isotropic material properties.

Acknowledgements

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Auxetic dome-shaped cellular structures

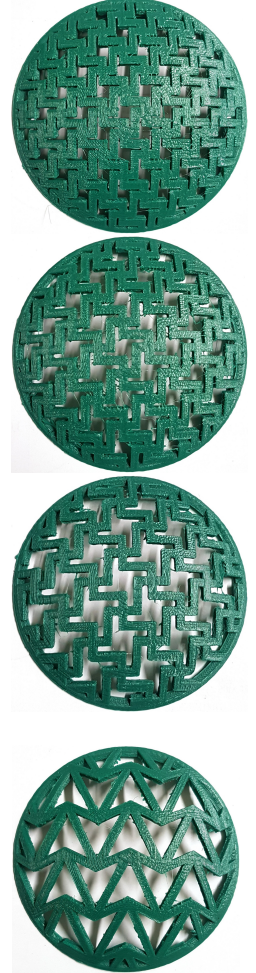
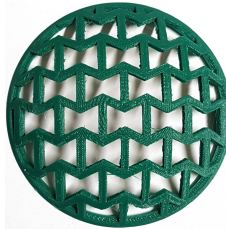
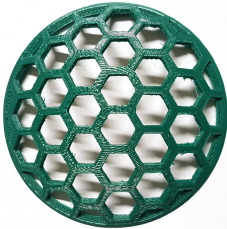
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This study describes the mechanical behaviour of three different auxetic cellular geometries (butterfly, cross-chiral and arrow-head) in a spherical (dome-shaped) space. We investigate the stiffness, failure strength and related mechanism from 3D printed PLA dome-shaped honeycomb samples under compressive loading, and compared the results with the ones from analogous conventional honeycomb configurations. We also investigate the effect of increasing the density of the honeycomb's cells on the overall mechanical properties. The behaviour of the 3D printed PLA material is first characterized by ASTM tensile and compression tests procedures. Domed-shaped honeycomb structures are then tested under compressive loading. The 3D printed PLA show a lower stiffness than the one exhibited by traditional samples fabrication methods. The domed-shaped honeycombs however exhibit markedly different behaviours highly dependent on the density of its cells, and also related to the auxetic geometries used in this work. This investigation opens up a new field of research related to the capability of 3D printing auxetic structures in curved and spherical domains.



Shape memory in magneto-auxetic systems

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It is shown that magneto-auxetic systems can exhibit both ferromagnetic and shape memory behaviour. In this work, the effect which the magnetic memory has on the magnetocaloric effect (MCE) exhibited by magneto-auxetic systems [1] in the vicinity of room temperature is discussed. Magneto-auxetic systems represent a class of metamaterials having magnetic insertions embedded within a non-magnetic matrix. In the model under consideration, the aforementioned non-magnetic matrix is represented by rotating squares with magnetic insertions in their centres. The magnetic memory is described by means of a correlation function between magnetic domains at different times.

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Hierarchical systems with tunable mechanical properties

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In this work, a model is proposed in order to investigate the deformation mechanism of a hierarchical system subjected to an external force. The proposed system consists of rotating rigid squares connected with each other by means of hinges. It is shown, that the behaviour of this structure may be solely controlled through the magnitude of the friction coefficient associated with the movement of the hinge connecting two adjacent rigid units. This result shows that structures corresponding to the same initial geometry may deform differently depending on the value of the friction coefficient, which in general can lead to a vast range of mechanical properties. In this work it is also shown that lower levels of the hierarchical system may open at a greater rate than it is the case for the higher levels, which result has not been reported in the case of the formerly studied perforated hierarchical materials.

Stability of extreme auxetic and incompressible elastic materials

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We investigate auxetic isotropic elastic materials with the Poisson's ratio of exactly -1 and isotropic materials with the Poisson's ratio of exactly 0.5 (incompressible). In both cases the energy loses positive definiteness, which can lead to the material instability. We consider both 2D and 3D formulations and demonstrate that under certain conditions the instability assumes the form of non-uniform displacement distribution.

Due to instability, the elastic materials with the Poisson's ratios of -1 or 0.5 cannot be manufactured (note the Poisson's ratios of the materials that are commonly believed to be incompressible are slightly smaller than 0.5). However the values of the Poisson's ratio can momentarily be altered when new fractures are formed under applied load. We present a newly developed theory showing that during the instantaneous process of fracture formation the fracture acts as a negative stiffness element; after the fracture is formed it immediately turns into a conventional fracture with usual positive stiffness/compliance characteristics. We demonstrate that such fractures are capable of momentarily bringing the Poisson's ratio of nearly incompressible material to 0.5 . This instantaneously turns the material into unstable. However in auxetics with the Poisson's ratio near -1 the extreme value of -1 still cannot be attained during the fracture formation. This proves the auxetic materials stable with respect to fracture formation.

On the thermo-mechanical properties of layered crystals

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DFT methodologies can be used to accurately simulate the mechanical properties and structural deformation of auxetic crystals. The same methods can also be employed to simulate the mechanical properties of theoretical crystals, giving a very good indication of the properties that such crystals would possess if synthesised.

The design of a crystal with the potential to exhibit specific thermo-mechanical properties should be based on a specific model which is known to lead to such properties. In this study, we will be focusing on the 'egg-rack' model proposed by Grima, which has been shown to exhibit a negative Poisson's ratio in one plane, accompanied by a giant positive Poisson's ratio in the perpendicular planes.

Here, we will show that the 'egg-rack' model can also exhibit the much sought-after property of negative linear compressibility and that of negative thermal expansion. The Poisson's ratio and compressibility of Molecular crystals based on this model will be studied through DFT simulations. Furthermore, their thermal expansion will be explored through force-field based molecular dynamics methods.

The two-layer tubes-auxetics of cubic crystals

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We analyzed the features of effective Young's modulus and Poisson's ratio of the hollow two-layer cylindrical tubes made of cubic crystals with different stiffnesses. A model of a cylindrical hollow rod with curvilinear anisotropic elasticity was used for the analysis of the elastic properties of tubes. As a result, the analytical expressions for effective Young's modulus and Poisson's ratio of the hollow two-layer cylindrical tubes are obtained. Numerical analysis of these formulas showed that the effect of one component of the tube to other is essential for two-layer tubular composite because of the stress-strain coupling. An example of a two-layer tube consisting of cubic crystals $\text{Sm}_{0.75}\text{Tm}_{0.25}\text{S}$ and Ca, as well as distribution of effective Poisson's ratios $\nu_{rz}(r)$, $\nu_{\varphi z}(r)$ of such layered tube are shown in Fig. 1. As it is seen from Fig.1a the entire volume of two-layer tube is auxetic for $\nu_{\varphi z}(r)$, and Poisson's ratio quickly reaches the value -1.56 on the inner surface of the layered tube (prior to the formation of two-layer tube the inner layer from Ca generally is not auxetics!). Poisson's ratio $\nu_{\varphi z}(r)$ changes only slightly in the outer layer 2 (Fig.1a). Poisson's ratio $\nu_{rz}(r)$ is positive in the inner layer 1 of two-layer tube and negative in the outer layer 2 (Fig.1b). Numerical analysis with other cubic materials showed that combining auxetics and nonauxetics in layered tubes allows to obtain a strong increase or decrease of auxeticity (degree of positive or negative Poisson's ratio) depending on order of layers stacking.

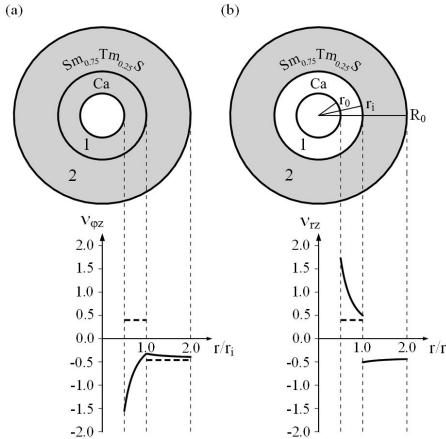


Figure 1. The cross-section of a two-layer tube of which the outer layer 2 is filled auxetics $\text{Sm}_{0.75}\text{Tm}_{0.25}\text{S}$ and the inner layer 1 is filled nonauxetics Ca. Fig.1a characterizes the distribution of effective Poisson's ratio $\nu_{\varphi z}(r)$, and Fig.1b characterizes effective Poisson's ratio $\nu_{rz}(r)$. Layers with a negative effective Poisson's ratio are painted gray, distribution of Poisson's ratios in separated single-layer tubes are indicated by dotted lines.

Acknowledgements

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Some recent advances in negative materials and structures

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In recent years there have been various developments in the field of 'negative materials and structures', including ones which exhibit a negative Poisson's ratio (auxetic, a term first proposed by K.E. Evans a quarter of a century ago), negative thermal expansion and/or negative compressibility. This paper will look into some of the more recent developments made in this field by the University of Malta group with particular emphasis on materials and structures with tailor-made 'negative' properties.

The effect of the density and the curvature of the walls on the elastic moduli of a new auxetic cell structure by a refined model

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The sandwich materials experiencing significant growth in both applications using , that technology in implementing them. They are of interest for applications that demand both strength and lightness, including transportation, marine, nautical, aeronautical, aerospace, sports, civil engineering and the military. It is interesting to know their mechanical properties to predict and calculate their behavior in specific environments. The properties of a solid cell depend not only on constituent materials, but also of the geometry of the cell. This paper is devoted to analytical and numerical modeling of elastic properties (Young's modulus, shear modulus and Poisson's ratio) of a new concept of honeycomb structure with a negative Poisson's ratio in the plane. Fig.1 [1]. The purpose of this concept is the presence of a curved base wall, we explore the solution based on the elasticity theory to calculate the Young's moduli and Poisson's ratio in the plane of the auxetic honeycomb structure with curved base wall according to the geometrical and mechanical parameters under axial loading taking into account all deferent combinations of stresses in the wall [2,3].

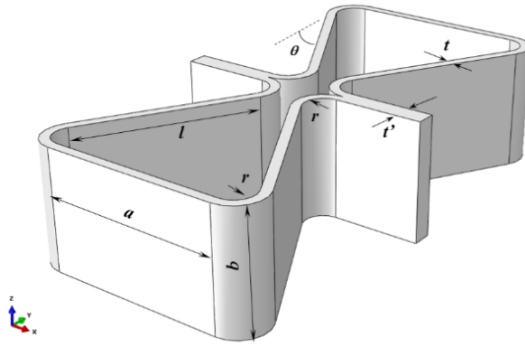


Figure 1. New design of the auxetic cell.

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Nanowire stretching by Non-equilibrium Molecular Dynamics.

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The elastic properties of crystalline and polycrystalline materials have been the subject of practical interest over many centuries. This subject was placed on a firm theoretical footing by Navier, Cauchy and Poisson. The strengths and failure mechanisms of solids under applied stress is an important aspect of this topic. In recent years this has extended to metallic nanowires used in electronics and micro-machine (MEMS) devices. The electronic and mechanical properties (e.g., their tensile strength and failure under uniaxial tension) of a given nanowire determine their suitability for particular applications. Large surface-to-volume ratios and other scale effects can mean that the mechanical response to straining of systems of nanoscale dimensions can be quite different to those of the same shape and chemical composition with macroscopic size. It is therefore necessary to make specific studies of such small scale systems rather than use predictions based on the classical (macroscopic) theory traditionally employed in engineering design, and referred to above.

The mechanism by which nanoscale wires of cross-sectional width of ~ 1 nm deform and break under tension can be quite different from those which are $l \sim 1$ μm or greater across in which sliding and deformation takes place predominantly by sliding at strain boundaries (just as with glassy systems the inhomogeneity of the local structure leads to a heterogeneous stress and strain distribution). Nanowires are to a large extent single crystals which cannot deform under stress by this mechanism.

The mechanical properties of Young's modulus and Poisson's ratio of a Lennard-Jones model nanowire are calculated as a function of a time dependent stretching along its axis, using a novel Non-equilibrium Molecular Dynamics (NEMD) procedure. The effects of strain rate are investigated. The mechanical properties are found to be strongly time-dependent straight from the start of the pulling process. The speed at which the wire is pulled has a major effect on the failure mechanism.

The deformation structures of the nanowire are presented in the form of atom assembly projections, and time traces of mechanical and thermodynamic properties as a function of strain.

Auxeticity due to elastic instabilities

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Elastic instabilities are usually deleterious and needed to prevent. In this study, we use elastic instabilities as helpful mechanisms to show auxeticity. Firstly, using atomistic simulations we show that some face-centered-cubic metals under tensile loading exhibit a large value of negative Poisson's ratio as the applied strain beyond a critical strain. This auxetic phenomenon is associated with the Born-Hill elastic instability. In addition, using atomistic simulation as well as finite element method calculation, we show that periodic porous metallic structures can also exhibit auxeticity at finite strains. Another elastic instability mechanism, Euler buckling of the microscopic elements leads to the auxetic behavior of the porous metallic structures.

Deformation behavior of auxetic quadruple helix yarns under tension

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Quadruple helix yarn (QHY) is a novel kind of 4-ply yarn with a special configuration and auxetic mechanism, where two elastic filaments and two high modulus filaments are employed to achieve the negative Poisson's ratio (NPR) behavior (Fig. 1) [1]. Compared with the helical auxetic yarn (HAY) which is based on a double helix geometry [2], the 4-ply helix structure is more stable so that twist regularity of the auxetic yarn could be improved. In the previous research, auxeticity of the HAYs was generally assessed in the axial elongation [3,4]. This paper presents a detailed optical microscopy study to investigate the changes in the internal structure of QHY leading to auxetic behavior under different axial strains. By measuring the cross-sectional parameters (Fig. 2(b) and (c)) and assessing the migration behavior of constituent yarns in the QHY from series of cross-sectional images (Fig. 3), it is validated that auxetic behavior inside the QHY (Fig 2(a)) is generated by the interplay between the soft yarns and the stiff yarns. During the axial extension, the migration of stiff yarns initially induced an increase in maximal diameter of the auxetic yarn, but further increase in the axial extension eventually led to a slow reduction in yarn diameter (Fig. 2(b)). By comparing different QHY samples which were fabricated with two types of stiff yarns and the same kind of soft yarn, it was found that tensile modulus of stiff yarn plays an important role in producing a high NPR.

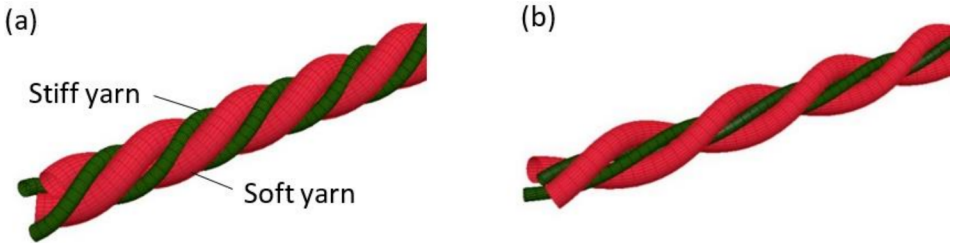


Figure 1. (a) QHY geometry at rest; (b) QHY under tension.

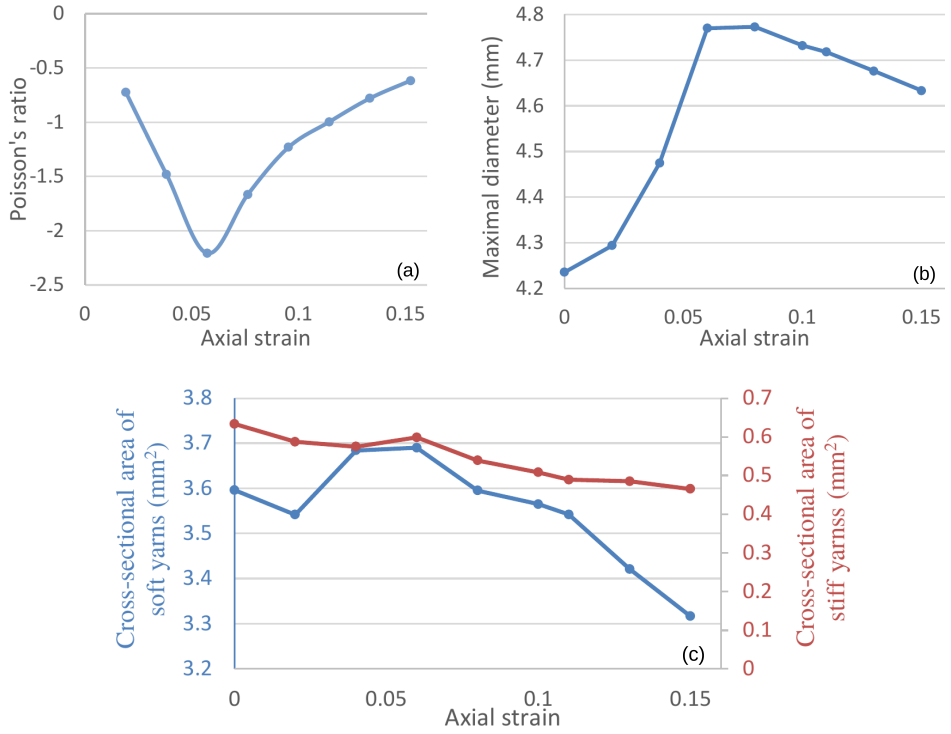


Figure 2. (a) Poisson's ratio-strain curve of QHY; (b) Maximal diameter of QHY as a function of axial strain; (c) Cross-section area of soft yarns and stiff yarns as a function of axial strain.

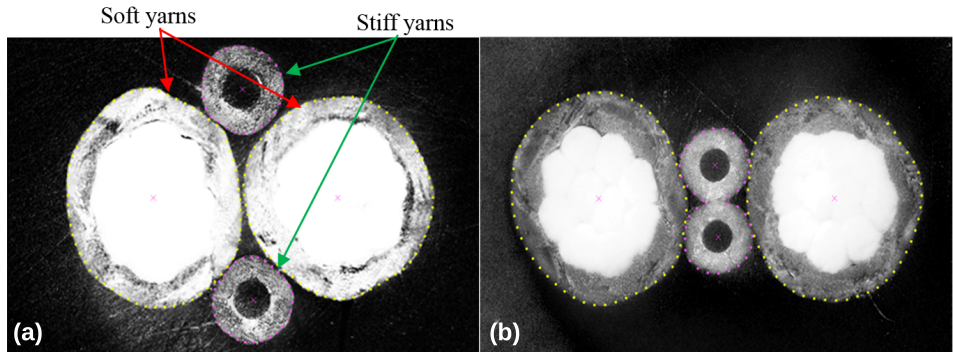


Figure 3. Cross-sectional image of QHY sample (a) at rest; (b) at strain of 0.11.

Acknowledgement

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Elastic properties of Yukawa systems with nanochannels

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Monte Carlo simulations in the isothermal-isobaric ensemble [1] of the modified Yukawa crystals [2] have been performed. Effects of introduction narrow channels filled by particles interacting via hard potential to Yukawa crystals have been investigated. The analysis of elastic properties of studied crystals has shown a relevant influence of the size of nanochannels on the value of Poisson's ratio [3] in main crystallographic directions.

In particular, presence of nanochannels in the direction [001] implies that the auxeticity in [110][1-10] direction is almost doubled, with respect to the system without nanochannels. The value of Poisson's ratio in this direction changes from $-0.15(2)$ to $-0.29(3)$ [4]. The linear relationship between the Poisson's ratio and concentration of particles filling channels in the system has been observed.

Acknowledgement

Part of the calculations was performed at the Poznań Computing and Networking Center (PCSS).

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The molecular dynamics methods for confined systems: thermal conductivity of liquid argon in nano-channels

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The understanding of mechanical properties of confined fluids is crucial for modeling and manipulating of systems in nano-scale. In this context, it seems interesting to ask a question, whether such systems could have auxetic properties. The answer to this question requires an appropriate research methodology to study nano-scale systems, which is still developed poorly. In this work we try to develop and apply some known methods to study physical properties of nano-scale systems.

In the present study, calculations of thermal conductivity of liquid argon in round and square nano-channels have been performed using two independent methods, the Green-Kubo approach [1,2] in equilibrium molecular dynamics simulations and the Müller-Plathe method [3] in non-equilibrium molecular dynamics simulations. The Lennard-Jones potential has been employed to model interatomic interactions.

The study shows that thermal conductivity increases with the cross-sectional area of the nano-channel until it reaches bulk values for some characteristic size of channel that depends strongly on density. This characteristic size varies from 5 nm (at 678 kg/m³) to 11 nm (at 1186 kg/m³) [4]. It is worth to note the good agreement of the computed thermal conductivities of liquid argon over a wide density range with the experimental data for bulk systems [5].

Acknowledgement

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Computational modeling of thermoauxetic composite structures

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Mechanical properties of auxetic materials have already been investigated for many years, however their thermal properties are studied less frequently. The impact of temperature on mechanical properties of materials is very well-known fact [1,2] that should be considered in the case of designing new constructions and composite materials. Recently, the influence of temperature on elastic properties of fibrous composite has been presented [3]. In this paper an analysis of mechanical properties of selected composites is presented. The geometries of composites structures are based on typical auxetic shapes. The resultant composites exhibit effective Poisson's ratio that changes from negative to positive values according to temperature applied (see Fig. 1).

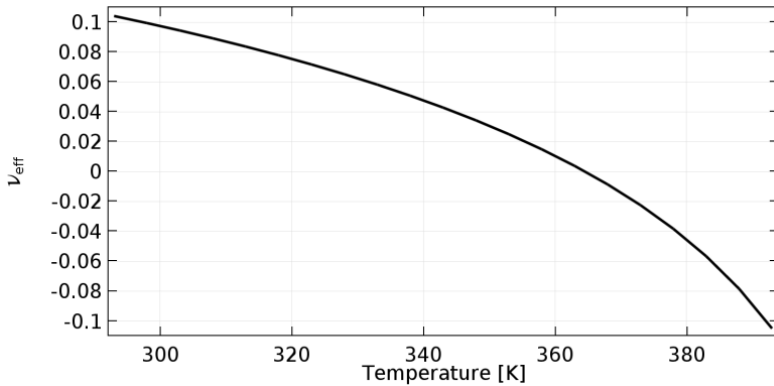


Figure 1. Effective Poisson's Ratio as a function of temperature.

Acknowledgements

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Sign reversal of the Hall coefficient in three-dimensional metamaterials

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In 2009, Briane and Milton have shown theoretically that the effective Hall coefficient of a metamaterial can be negative with respect to the Hall coefficients of its constituents [1]. They proposed an isotropic three-constituent structure based on interlinked tori. Last year, we have shown by numerical simulations that the same effect can also be obtained from single-constituent metamaterials [2]. This means that a metamaterial made of an n-doped semiconductor can effectively act as a p-doped semiconductor and vice versa.

Here, we report on the fabrication and characterization of such metamaterials [3]. In order to measure their Hall coefficient, we fabricate Hall bars composed of $11 \times 5 \times 1$ metamaterial unit cells. The lattice constant is typically around 100 μm . In a first step, we write polymer structures which serve as scaffolds using three-dimensional laser lithography. Next, we coat the samples conformally with a layer of n-type ZnO using atomic layer deposition. Finally, in order to obtain Ohmic contacts, we deposit layers of titanium and gold using electron-beam evaporation. Our measurements are performed using a home-built probe station. The magnetic field is imposed using a movable permanent magnet.

Our experimental results confirm the sign reversal expected from theory. Moreover, we find that one can tune the Hall coefficient continuously by changing a geometrical displacement parameter. Corresponding numerical simulations are in excellent agreement.

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The Effects of Poisson's Ratio on the Mechanical Behaviour of Embedded System in an Elastic Matrix

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Soft materials with embedded stiffer layers are increasingly used in medical and sport engineering. A detailed understanding of the mechanical behaviours of such a system is crucial to the structural integrity, functional performance and reliability of the embedded systems. The deformation of embedded layers under uniform or localised loading conditions is different from traditional layered composites. In this work, a new modelling method of embedded 2D structures was developed and correlated with analytical solution at different strain levels and loading modes. A parametric program was used to generate different distributed structures. The resistance of soft material systems under localised loading conditions with matrix of both positive and negative Poisson's ratio values was systematically studied. The influence of auxeticity on an embedded system is highly thickness and depth dependent. The potential use of modelling approach in designing soft material system with enhanced protection and compliance is also discussed.

An auxetic structure with NTE characteristic

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SIM University, Singapore

A 2D array of ring-based structure is proposed herein. This ring array can be shown to exhibit auxetic properties as well as partial negative thermal expansion (NTE). This type of structure is then extended to a 3D array that also exhibits partial NTE characteristics.

Tension and torsion nanomicrotubes with cubic cylindrical anisotropy

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Model of a hollow rod with a cylindrical anisotropy to describe the mechanical properties of nanotubes and microtubes is proposed in [1-3]. In these articles the problem of stretching and twisting of nano/microtubes with cubic, hexagonal and rhombohedral cylindrical anisotropy are considered in Saint-Venant's approach. It was assumed that the nano/microtubes were obtained by rolling the crystal planes (001). In this work, the problem of stretching and twisting nano/microtubes with cubic cylindrical anisotropy obtained by rolling the crystal planes (011), are considered in Saint-Venant's approach. A result of analyzing the analytical expressions of Young's modulus and Poisson's ratio taking into account the chirality angle (the angle between the crystallographic axis and the axis of elongated tube) are obtained. Numerical analysis was performed for the nano/microtubes from Al crystals, Fe crystal and $\text{Sm}_{0.65}\text{La}_{0.35}\text{S}$ alloy, which are nonauxetics, partial auxetics and complete auxetics respectively. Analysis showed that the nano/microtubes from Al and Fe will have a negative Poisson's ratio. Poisson's ratio for the nano/microtubes from $\text{Sm}_{0.65}\text{La}_{0.35}\text{S}$ alloy remains negative in all chirality angles and thickness of tubes. Young's modulus for nano/microtubes of these materials at a fixed chirality angle weakly depends on the thickness of the tubes. Young's modulus may change several times as a function of chirality angle in the case of a fixed thickness of the tube.

Acknowledgements

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Friction of confined particle films under external load and shear by Non-equilibrium Molecular Dynamics

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Controlling friction between contacts acting on a small lengthscale has become a pressing issue in a number of fields involving miniaturized mechanical components. Experiments carried out on atomistically flat surfaces have shown that on this scale the friction laws can be quite different to the classical ones of Coulomb and Amontons. Notably, the friction coefficient increases with relative sliding speed and there can be periodic variations of the sliding force arising from the traversal of the two crystalline surfaces over each other.

In some tribological applications the pressures applied in the contact zone can be several GPa so that any confined film can be in a solid or semi-solid state. Investigations of the impact of applied pressure and shear rate on the confined film states of the atomic system (condensed phase argon) are presented. Boundary-driven simulations mimicking a typical experimental arrangement were carried out with thermostatted sliding walls as a means of initiating and sustaining shear flow.

The regions of different steady states has been established. The friction coefficient, and friction force maps are obtained and interpreted in the light of the accompanying non-equilibrium phase diagram. Stick-Slip behavior is observed which is shown to be accompanied by a novel recurrent in-plane melting of crystalline layers of the confined sample which form parallel to the wall. The so-called Plug-Slip (PS) steady state is shown to exhibit particularly anomalous frictional behavior, for example the friction coefficient can decrease with increasing load, which is counter intuitive behavior and contrary to macroscopic friction laws. It is observed that the PS frictional behavior can be state point history dependent to varying extents depending on the part of non-equilibrium phase diagram considered. For example, it is shown that it is possible by increasing the pressure first and then the wall speed, to ‘lock in’ to much higher sliding speeds very low friction states which normally appear at low sliding speeds only.

Non-equilibrium phase behavior of confined molecular films in low-speed regime

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Friction is an extremely complex physical process, and its origin can vary from system to system. Contact topology, molecular interactions and mechanisms of energy dissipation can vary with material and physical conditions, such as whether the contact is dry or lubricated by an intervening liquid or solid.

When there is a molecularly thin third material acting as a lubricant between the two sliding surfaces, experiment, and Non-equilibrium Molecular Dynamics (NEMD) simulations have shown that the instantaneous friction coefficient can vary with time in a repetitive way for relatively low sliding speeds [1]. This ‘Stick-Slip’ (SK-SL) behavior has been attributed to a recurrent solidification and shear-induced melting of the confined material during the sliding process. NEMD simulations have also revealed a non-equilibrium steady state of the confined system, which under pressure and sliding speed below 50 m/s can transform into a non-flowing plug with slip at the walls, which we have called the ‘Plug Slip’ (PS) state [2]. Some of the non-equilibrium steady states have been currently observed experimentally [3-5], especially Plug-Slip and Central Localization states using a novel methodology, based on the use of phosphorescence imaging. It can be shown that the friction force corresponding to Stick-Slip and Plug-Slip behavior does not depend monotonically on applied load. Moreover, there are regions where the value of friction decreases with increasing load which is a counterintuitive result [6]. Frictional behavior on the molecular scale can be quite different to that observed for macroscopic objects (which are well described by the classical laws of friction).

Both SK-SL and PS steady states can occur in a range of low sliding speed (usually below 50 m/s). In this presentation attention is especially paid to the low-speed regime ($v < 5$ m/s) and the $v \rightarrow 0$ limit. The steady states of strongly confined systems under variable load and shearing rate (within low-speed regime) were carried out using NEMD simulations. The friction coefficient, and friction force maps obtained are discussed in the light of the accompanying non-equilibrium phase diagram.

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Tri-layered auxetic scaffold for bone regeneration

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Auxetic materials have unique property of possessing a negative Poisson's ratio, thus displaying the property of lateral contraction during longitudinal compression, and lateral expansion during longitudinal expansion [1-3]. This unusual mechanical behaviour is said to result in improved mechanical properties of the scaffold by increasing its energy absorption, and improving its fracture toughness. These properties are beneficial since they are expected to provide loading and unloading of cells, hence, improving the behaviour of bone cells in terms of increasing their proliferative capacity, and their ability to mineralise bone. This study presents the fabrication of a tri-layered scaffold for bone tissue engineering that displays such counter-intuitive mechanical behaviour. The process of solvent casting is used to form porous scaffolds made from a composite of chitosan, polycaprolactone, and hydroxyapatite, which respectively set in a tri-layered fashion. Auxetic geometries developed theoretically in previous research [4] are laser cut onto these scaffolds, which are then tested to evaluate their Poisson's ratios. This study thus aims to achieve scaffolds that mimic the natural properties of bone, thus aiding in the improved repair and regeneration of bones.

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Effective Young's modulus and Poisson's ratio of the thermoelastic normal and auxetic plate determined from the extended thermodynamical model

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The problem of effectiveness of material coefficients when materials are subjected to dynamical processes is very important if they are to be used to make parts of devices or constructions which should work very precisely. To avoid any inaccuracy constructing them, that problem should be exactly recognized. The values of those coefficients depend on specific space and time scales which the parts of devices are working in. The presentation deals with computer simulations of the above problems within the normal and auxetic states concerning a vibrating thermoelastic plate of finite extent which the thermal relaxation occurs in.

Failure of classical elasticity in auxetic foams

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Poisson's ratio, ν , was measured for four materials, two auxetic foams, a conventional soft foam, and a rubbery polymer. We find that for the latter two materials, having $\nu \geq 0.2$, the experimental determinations of Poisson's ratio are in good agreement with values calculated from the shear and tensile moduli using the equations of classical elasticity. However, for the two auxetic foams, the equations of classical elasticity give values significantly different from the measured ν . We interpret these results based on a recently published analysis of the bounds on Poisson's ratio, which demonstrated that for materials with $\nu < 0.2$, while physically possible, cannot obey the classical theory of elasticity.

Poisson's ratio of the DC phase of hard dimers with arrays of nanochannels

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Elastic properties of the f.c.c. degenerate crystalline (DC) phase of homonuclear hard dimers with arrays of nanochannels filled by identical hard spheres are studied by Monte Carlo simulations. The applied method can be used to determine Poisson's ratio in all directions for crystals of arbitrary symmetry [1]. The periodic array of channels oriented along one of the directions [001], [110], and [111] are considered. The spheres forming dimers have the diameter σ which can be different from the diameter σ' of spheres filling the channels. It is shown that, by modifying the ratio σ'/σ , one can qualitatively modify the Poisson's ratio of the system. In particular, one can obtain partial auxetics (i.e. systems with negative Poisson's ratio in some directions). Explicit analytic formulae expressing Poisson's ratio through elastic compliances in main directions are also given for the studied structures.

Acknowledgments

Part of the simulations was performed at the Poznań Supercomputing and Networking Center.

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Computational modeling of auxetic structures

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Computational modelling and simulations offer a promising way for development of new complex auxetic geometries which may be fabricated using additive manufacturing technologies. The response of the auxetic structure under particular loading conditions can be tailored through changes of the cellular auxetic structure geometry using validated material properties and optimisation techniques to achieve the best desired mechanical response [1].

This work presents an analysis of the auxetic structures made of the Ti-6Al-4V powder by the selective electron-beam melting method (SEBM) at the Institute of Materials Science and Technology (WTM), University of Erlangen-Nürnberg, Germany [2]. Quasi-static compressive testing of auxetic specimens in two orthogonal directions was performed to determine their basic mechanical behaviour. The results from experimental testing were used to validate the developed discrete lattice computational models as well as homogenised computational models based on the crushable foam material model using the finite element code LS-Dyna. Validated discrete computational models were used for further optimisation of the auxetic structure geometry to obtain user defined response during compression loading by applying a functionally graded porosity principle (Fig. 1).

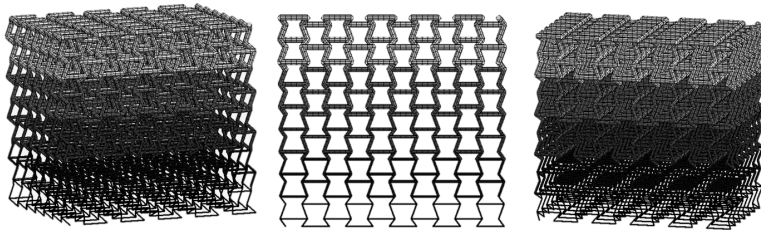


Figure 1. Numerical model of auxetic structure with functionally graded porosity.

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Wave propagation in materials with negative moduli

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Recently a possibility of materials with microstructure that creates an effect of negative stiffness has been theoretically demonstrated. When the elastic energy is no longer positive-definite such materials are inherently unstable, yet they can be stabilised by appropriately chosen boundary conditions. Understanding the possibility and characteristics of wave propagation in such materials is important as it can provide means of monitoring the internal state and stability.

Isotropic materials with negative shear of Young's modulus cannot support elastic wave propagation. However, there are cases when the effect of negative stiffness is provided by internal rotations of non-spherical constituents in the presence of external uniaxial compression. In these cases the negative stiffness relates shear force and the rotation. As rotations are involved they form additional degrees of freedom and consequently lead to the introduction of a Cosserat continuum. We concentrate on the simplest case of isotropic Cosserat continuum, governed by six independent moduli: two conventional Lamé constants and four Cosserat moduli controlling the relationship between the stress and moment stress on the one hand and the internal rotations and their gradients on the other. The (infinitesimal) rotation of non-spherical particles creates the effect of negative Cosserat shear modulus that is the modulus that relates the internal (particle) rotations with non-symmetric parts of stress tensor.

We demonstrate that there exists a range of values of the negative Cosserat shear modulus at which the wave propagation is still possible such that all four types of waves (p-wave, two shear waves and a twist wave) exist. Furthermore, while in the conventional isotropic Cosserat continuum the twist wave and one of the shear waves exist only at high frequencies, higher than a certain threshold frequency, the presence of the negative modulus removes this threshold. Therefore the negative modulus of admissible values makes all four waves exist in all frequencies. Obviously the lengths of the propagating waves must be much larger than the microstructural sizes of the material, which are the sizes of the rotating constituencies. We demonstrate that these sizes are commensurate with the Cosserat characteristic lengths and determine the frequencies at which the waves can propagate.

Elasticity of mono- and polydisperse crystals of hard-core repulsive Yukawa particles

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Elastic constants of mono- and polydisperse Yukawa crystals have been determined using Monte Carlo simulations in isobaric-isothermal ensemble with variable-shape simulation box [1]. The calculations were performed, for both two-dimensional (2D) hexagonal and three-dimensional (3D) face centered cubic (fcc) crystals, in which particles interact via hard-core repulsive Yukawa potential [2,3]. The influence of changing the contact potential (ε), the Debye screening length (κ^{-1}), and polydispersity parameter (δ) on the elastic properties of those systems have been studied.

Simulations show that elastic moduli of 2D crystal increase with density and/or the value of contact potential. The Debye screening length has significant influence on the rate of growth of the elastic moduli [4]. Moreover, it was shown that in the case of 2D Yukawa crystal the size polydispersity of particles has an essential impact on the elastic moduli, especially on the shear modulus [4]. However, auxetic properties have not been observed in the studied 2D systems. In the 3D fcc Yukawa crystal it has been observed partial auxeticity for $[110][\bar{1}\bar{1}0]$ orientation [5]. The present study shows that the value of Poisson's ratio in this direction is negative and depends on the polydispersity of the particle size and the Debye screening length. An increase of δ and/or κ^{-1} leads to a further decrease of the Poisson's ratio and amplification of auxeticity for the $[110][\bar{1}\bar{1}0]$ orientation.

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The calculations were partially performed at Poznań Supercomputing and Networking Center (PCSS).

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Molecular simulation as a guide for potential auxetic materials

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The last years have witnessed the emergence of molecular simulation as a guide for the synthesis of new materials. It is thus an appropriate approach to predict potential auxetic candidates prior to their synthesis. However the lack of simple existing auxetic systems at the molecular level means that the crucial step of validation cannot be carried out. A specific procedure must therefore be established. The actual transition from the structure of a molecule to the final functionality of a material is far from straightforward. To describe real systems, a series of models is required. Models must first be chosen to efficiently describe the system of interest. We thus propose to calibrate our strategy first on isotropic compounds such as polymers, or organic glasses. The procedure is then applied to anisotropic materials, such as liquid crystals. The agreement with experimental behaviour allowed us to extrapolate the procedure to potentially auxetic compounds, thus offering great opportunities to reveal auxetic properties prior to the synthesis of the molecules.

Isotropic and continuous planar auxetics from hard star-shaped inclusions – numerics and experiment

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Recently, it was shown [1] that by introducing an ordered pattern of hard elliptic inclusions into a continuous matrix (of any Poisson's ratio) one can obtain structures which are partially auxetic [2], i.e. exhibit negative Poisson's ratio in some directions. In this work isotropic structures similar to the one presented in Fig. 1 are considered.

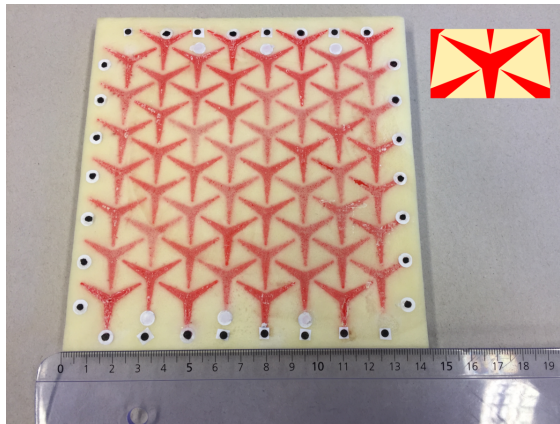


Figure 1. Exemplary structure made of PU foam (white) and 3D-printed hard inclusions (red). The inset presents the unit cell.

Extensive numerical studies of samples of the geometry illustrated in Fig. 1 were performed for various material properties and geometry parameters. These investigations resulted in conclusion that it is possible to obtain isotropic auxetics using (sufficiently) hard inclusions of proper shape and size. In particular, the sample shown in Fig. 1 was predicted to exhibit negative Poisson's ratio close to -0.07 . The latter value was confirmed in separate, experimental studies.

It is worth to stress the following two facts:

- (i) the considered structures are built of conventional materials, e.g. rigid non-auxetic inclusions and a foam of (slightly) positive Poisson's ratio, and
- (ii) the Young's modulus of the resulting auxetics can be arbitrarily large if the inclusions are hard enough.

Acknowledgements

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Sign reversal of the thermal expansion coefficient in metamaterials fabricated via three-dimensional dip-in direct laser writing

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Years ago, Lakes showed theoretically that the thermal length-expansion coefficient of metamaterials composed of two constituents and air voids within is principally unbounded [1]. This includes the possibility of negative thermal length expansion from positive constituents. Here, we design, fabricate, and characterize corresponding two-component three-dimensional micro-structured polymer metamaterials made by gray-tone three-dimensional laser lithography. The different local exposure doses lead to different polymer cross-linking densities, hence different mechanical properties, hence different positive length-expansion coefficients. We characterize the metamaterials by optical microscopy imaging combined with detailed cross-correlation analysis of these images, allowing us to directly measure the temperature-induced displacement-vector field on a sub-pixel and sub-wavelength spatial scale. We find that the thermal length-expansion coefficient can be tuned by geometry from positive to zero to negative values. The cross-correlation images indicate a nearly homogeneous and isotropic behavior—in good agreement with numerical simulations.

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The application of auxetic materials in tissue engineering

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Tissue engineering scaffolds for regenerative medicine are required to withstand a variety of loading conditions, to match target tissue attributes, to support and stimulate cell growth, and to define the ultimate shape of the new tissue. Natural biological tissues are now known to display auxetic characteristics (the material becomes thicker, rather than thinner, when stretched), corresponding to negative values of Poisson's ratio. These include certain forms of skin [1,2], artery [3], tendon [4], early stage amphibian embryo tissue [5] and, possibly, cancellous bone [6]. Natural biomaterials can also display gradient and/or anisotropic structure and properties. Mechanical stimulation of the scaffold promotes cell proliferation and a recent study indicates enhanced proliferation may occur in an auxetic polyurethane (PU) foam scaffold [7]. Auxetic porous materials facilitate mass transport [8] and, therefore, the potential for optimal flow or delivery of nutrients, metabolic wastes and therapeutic agents. Furthermore porous materials have the potential to enable migration of cells into the scaffold thus supporting improved tissue growth. For these reasons, the development of porous auxetic materials promises to deliver improved next-generation tissue engineering scaffolds.

Here we report further development of recent work on imparting gradient structure and properties into PU foams, together with an investigation into the growth of rat mesenchymal stem cells (rMSC) in open cell PU foams, and on the surface of an auxetic warp knit fabric.

Large area planar foams having distinct regions of isotropic auxetic behaviour and highly anisotropic foam having positive and negative Poisson's ratios under in-plane tension and compression, respectively, have been produced. This has been

achieved by adapting the 'method of pins' in combination with the established thermo-mechanical conversion of conventional parent foam. Previously, the use of pins has been developed for longitudinal and radially-gradient foams [9], and in this work the pins provide localised in-plane constraint (compression or extension).

To produce auxetic foam samples for the cell growth investigation, P80 PU foams (Custom Foams) with 80 pores per inch ('ppi') before conversion were manually compressed to one third of their initial volume in 23mm×23mm×45mm moulds and heated in three stages: 190°C for 15 minutes, 190°C for 10 minutes, then 100°C for a further 10 minutes. The foam was removed from the oven and mould between each heating stage and gently stretched by hand, then reinserted into the mould and oven, to reduce rib adhesion and surface creasing. The auxetic fabric was produced as described in ref [10] (fabric #4). The foam and fabric were cut into 5mm×5mm×2.5mm and 10mm×5mm×1mm cuboids, respectively, and sterilised in 100% ethanol, washed in PBS and cell culture media in a laminar flow hood.

Each cuboid of foam and fabric was coated with 50µg/ml of fibronectin, seeded with 6.4×10^3 rMSC cells/mm³, and cultured under standard conditions for up to 3 weeks in low-adhesion plates. Following cell culture for 1 or 3 weeks, samples were histologically processed and 4µm sections were stained for morphological analysis using a Haematoxylin and Eosin (H & E) stain. Duplicate samples were snap frozen, freeze dried, and coated with 24nm of gold, for scanning electron microscopy (SEM) examination.

Sixty micron sections stained with H & E and analysed by SEM were used to observe the pore structure and localization of cells in the auxetic foam. Hoechst 3342 staining and Alamar blue were used to examine cell viability.

Histological results showed the presence of clusters of cells within the auxetic foam and fabric samples at 1 week, which increased at 3 weeks. This was also confirmed by SEM which showed the presence of extracellular matrix forming bridges with the foam pores. The use of Sudan black and Hoechst 3342 enabled the visualization of normal cell nuclei and alamar blue demonstrated proliferation of cells within foams over the culture period.

In summary, rat mesenchymal stem cells were successfully grown within the auxetic foam and knit fabric samples, confirming both these materials have potential use in tissue engineering applications. The ability to impart gradient properties into the foam scaffold has been extended to large area foam sheets.

Acknowledgements

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Nonlinearity of elastic deformation and moderateness of strains as a factor explaining the auxeticity of material

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First the basic statements from the geometrical (kinematic) part of nonlinear theory of deformation of materials are formulated and commented. The starting point is the Truesdell's note [1, chapter IX, section 1] "it seems to be useful to introduce the displacements in mechanics if only both displacements and their gradients are small in some sense". Therefore the main statement is associated with the measure of deformation. The vector of displacement of the point-particle M is introduced as the quantity $\vec{OM} - \vec{OM}^* = \vec{R} - \vec{r} = \vec{u}(x_1, x_2, x_3)$, when the point M in the undeformed state passes after deformation into the point M^* , which is defined by the radius-vector $\vec{OM}^* = \vec{R} = (x_1 + \Delta x_1, x_2 + \Delta x_2, x_3 + \Delta x_3)$. Then a measure of deformation is introduced $u_m(x_1 + \Delta x_1, x_2 + \Delta x_2, x_3 + \Delta x_3) = u_m(x_1, x_2, x_3) + \frac{\partial u_m}{\partial x_k} \Delta x_k + \sum_{n=2}^{\infty} \frac{\partial^n u_m}{(\partial x_1)^{n_1}} \Delta x_1^{n_1}$, $n_1 + n_2 + n_3 = n$; in the representation above, the only linear approximation

$$u_m(x_1 + \Delta x_1, x_2 + \Delta x_2, x_3 + \Delta x_3) = u_m(x_1, x_2, x_3) + \frac{\partial u_m}{\partial x_k} \Delta x_k \quad (1)$$

is saved in mechanics. This linear approximation is used both the linear theory and the different nonlinear ones. Some other kinematic and kinetic notions are introduced and commented.

Further, the main facts from theory of universal deformations (uniform deformations, universal states) are described and commented as an important fragment of mechanics of materials. The universal deformations occupy the special place in the theory of elasticity just owing their universality. It consists in that the experimentally and analytically determined elastic constants in samples (in which the universal state is created) are true for all other deformed states both samples and any other pieces of material. It is accepted therefore that the special importance of universal states (their fundamentality) consists in possibility of their use in determination of the properties of materials from experiments. To realize the universal deformations, two conditions have to be fulfilled: 1. Uniformity of deformation must be independent from the choice of material. 2. Deformation of material must occur by only the surface loads. In the theory of infinitesimal deformations, the next types of universal deformations are studied: simple shear, simple (uniaxial) tension, uniform volume compression. In the linear theory of elasticity, the experiment with a sample, in which the simple shear is realized, allows to determine the shear modulus μ . The experiment with a sample, in which the uniaxial tension is realized, allows to determine the Young elastic modulus E and Poisson ratio ν . The

experiment with a sample, in which the volume compression is realized, allows to determine the elastic bulk modulus k . Also, in the theory of elasticity, the uniform states of two-axial non-symmetric tension, two-axial symmetric tension, uni-axial compression, pure shear are used. While being gone from the linear (two-constant) model of very small deformations to the model of moderate or finite deformations, the universal deformations allow to describe analytically and experimentally some new nonlinear phenomena. History of mechanics of materials fixed the experimental observation in XIX century by Coloumb, Wertheim, Poynting and Kelvin the nonlinear effects that occurred under simple shear. About one hundred years later, these effects were described analytically within the framework of the three-constant Mooney-Rivlin model. In this way, the necessity to consider briefly the basic modern models of nonlinear elastic deformation arises. They all are related to the hyperelastic models, based on introducing the elastic potentials. The two-constant Neo-Hookean model, three-constant Mooney-Rivlin model and Ogden model, five-constant Murnaghan model are described and commented. Further the Murnaghan model is considered more in details. The standard representation is used

$$W(\varepsilon_{ik}) = (1/2)\lambda(\varepsilon_{mm})^2 + \mu(\varepsilon_{ik})^2 + (1/3)A\varepsilon_{ik}\varepsilon_{im}\varepsilon_{km} + B(\varepsilon_{ik})^2\varepsilon_{mm} + (1/3)C(\varepsilon_{mm})^3, \quad (2)$$

where λ, μ are the Lamé elastic constants and A, B, C are the Murnaghan elastic constants. Then the universal states of simple shear, uniaxial tension, omniaxial compression are described analytically within the framework of Murnaghan model. The special attention is drawn to the uniaxial tension of the circular long cylinder. Here two unusual properties of elastic material are shown. A new nonlinear effect is revealed: the link among the stress in direction of tension σ_{11} and the lateral ε_{11} and transverse ε_{22} strains, which corresponds in the linear approximation to the Young's modulus E , is nonlinear in the case of moderate values of these strains. This effect is similar to the Poynting's and Kelvin's effects in the problem on universal deformation of simple shear, which state the nonlinear influence of the value of shear angle on the shear stress and the appearance of normal stresses, respectively. The second effect is associated with the values of ratio of the lateral strain to the transverse one, which corresponds in the linear approximation to the Poisson's ratio ν . It is also changed in the same range of values of the longitudinal strain ε_{11} . This is shown in Fig.1 that corresponds to polypropylene (left plot) and foam (right plot).

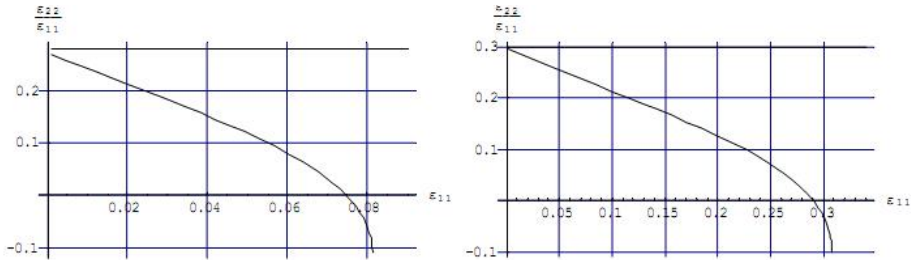


Figure 1. Poisson's ratio versus longitudinal strain (numerical).

The change is so essential that the value of this ratio changes the sign and becomes negative for the moderate strains. Thus, nonlinearity of elastic deformation in combination with the moderate strains describes the property of auxeticity of materials. This explains, for example, the auxeticity of foams, for which this property become apparent not for the small strains and therefore using the linear approximation is not correct. The numerical results are compared with two experimental data from [2] (Fig.2) and [3] (Fig.3, right plot).

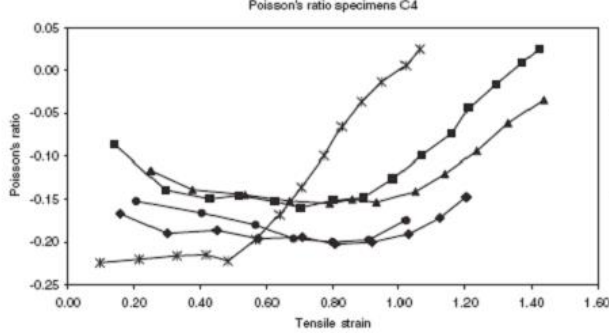


Figure 2. Poisson's ratio versus longitudinal strain (experimental).

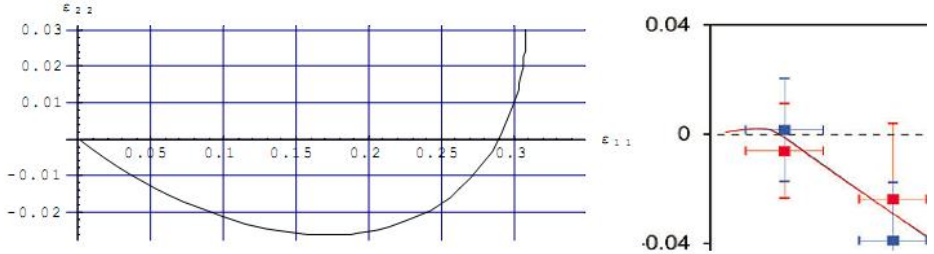


Figure 3. Transverse strain versus longitudinal strain.

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The effective coefficient of thermal expansion of material with auxetic inclusions

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We study thermo-elastic behavior of the hybrid materials with auxetic inclusions. To this end we analyze representative volume elements consisting of a large number of randomly positioned prismatic inclusions using the finite element method and determine the effective coefficient of thermal expansion and the average thermal stresses in constrained hybrid materials developed as a result of a uniform temperature change. We study the effect of Poisson's ratio, Young's modulus and the coefficient of thermal expansions of the inclusions on the effective coefficient of thermal expansion and thermal stresses. We demonstrate that the auxeticity of the inclusions can reduce thermal stresses, which is controlled by the values of the Poisson's ratio and the coefficient of thermal expansion of the inclusions and matrix. The negative coefficient of thermal expansion of the inclusions leads to further reduction in thermal stress.

Vibration properties of sandwich panel with folded plates core

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When materials are compressed along a particular axis the most common effect is their expansion in the transversal directions (materials with positive Poisson's ratio PR). Mechanical [1] and thermodynamical [2] models were found, which show the opposite behavior (negative PR): they shrink in transverse directions under longitudinal loading. When auxetic foams have been developed by Lakes [3] in 1987, it is known that materials and structures showing the anomalous behavior do exist in nature. Such a property, often referred to as auxeticity, occurs due to their particular internal structure and they deformation mechanism when their samples are uniaxially loaded (compressed or stretched).

Various re-entrant auxetic structures were introduced based on their shape. They were named: lozenge grids, sinusoidal ligaments, square grids, double arrowhead, re-entrant stars and structurally hexagonal re-entrant honeycomb. More information on auxetic structures can be found in recent reviews, [e.g. 4]. Auxetic materials are being progressively employed in the development of novel products, especially in the fields of intelligent expandable actuators, shape morphing structures and minimally invasive implantable devices or as core or phase material of structures and panels [5].

Grima and co-authors [6] presented a novel class of two-dimensional periodic structures build of star-shaped units of different rotational symmetry which are connected together to form two-dimensional periodic structures which can be described as "connected stars".

Some papers on auxetic materials are related to dynamics properties of auxetics or composite with auxetic phases [7-13]. It was shown that most of auxetic structures are characterized by interesting structural and dynamic properties.

In this paper dynamic properties of a sandwich panels made of two face-sheets and auxetic or non-auxetic folded plates core structure are analysed in this study by computer simulations. The periodic structure of inner core is made of a folded plates. The cross-section of core has shape of periodic structure with re-entrant four-stars unit cell geometry (see Figure 1A).

Assuming harmonic motion of the structure we can write displacement vector in the form of

$$u(x, t) = u(x)e^{i\omega t} \quad (3)$$

and finally the Navier's equation of motion as

$$\rho\omega^2 u - \nabla \cdot \sigma = F \quad (4)$$

or

$$\rho\omega^2 - (\mu\nabla^2 u + (\lambda + \mu)\nabla(\nabla \cdot u)) = F \quad (5)$$

when linear constitutive equation is assumed. It may be viewed as an eigenvalue equation for the operator $(\mu \nabla^2 u + (\lambda + \mu) \nabla(\nabla \cdot u))$ with an eigenfunction $u(x)$ and $\rho \omega^2$ as an eigenvalue.

Calculating displacement field in the structure, one can determined a vibration characteristics of the structure. The load on some boundaries of structure causes vibration of the face sheets as well as the composite core. The response of the structure is measured by vibration transmission loss [7]. Vibration transmission loss (VTL) of structure one can calculate using following formula

$$\text{VTL} = 10 \log_{10} \frac{\iint_{Bi} (\omega u_3)^2 dB_i}{\iint_{Bt} (\omega u_3)^2 dB_t} \quad (6)$$

where Bi , Bt are boundaries where load is applied and on opposite site along load action, where load is transmitted. In considered case load is applied on top boundary of structure acting in z-direction.

Some numerical results are presented in Figure 1B-D. Figure 1B presents total displacement values of structure loaded on top boundaries of structure and fixed on left and right edges of structure. Figure 1C presents vibrations transmission loss of structure versus frequency (from 1 to 100 Hz) of harmonic load. Results are presented for different parameters of inner core structure (auxetic or non-auxetic). Figure 1D presents first twenty eigenfrequencies. Generally it is observed that presented structure's damping properties are greater (greater positive value of VTL or greater values of eigenfrequencies), when inner core structure are characterized by negative Poisson's ratio and frequency of applied load is greater (see Figure 1C and 1D). Thickness of shell panel structure is such that the volume of the material used in the structure construction is constant irrespective of other geometrical parameters.

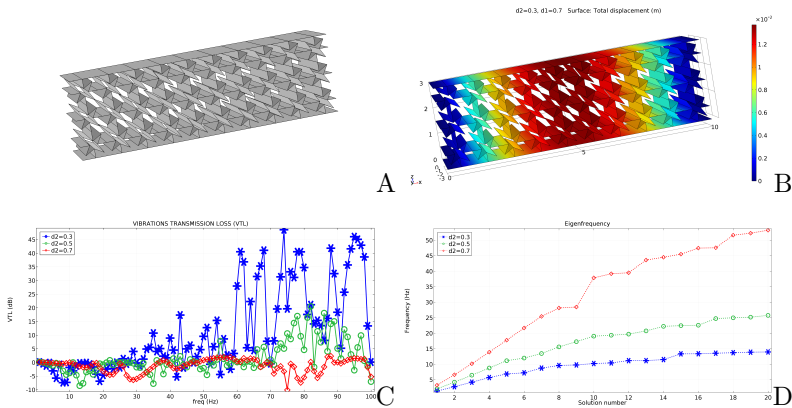


Figure 1. (A) Sandwich panel with re-entrant 4-star folded plates core, (B) deformation of panel, (C) TVL vs frequency, (D) eigenfrequencies for different structure parameters.

Acknowledgements

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Auxeticity of the Yukawa crystals with nanoslits and nanochannels

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Extensive Monte Carlo simulations in the isothermal-isobaric ensemble of nanocomposites in which particles interact by hard-core repulsive Yukawa potential [1,2] have been performed. The Poisson's ratio of material composed of periodically repeating sequences of the nanoslits or nanochannels filling by the hard spheres in Yukawa crystal is determined. The influence of the concentration of nanoslit or nanochannel particles in the system on the Poisson's ratio have been also studied.

Simulations of studied systems reveal strong changes of the Poisson's ratio caused by modification of the Yukawa crystal through introduction of monoatomic nanoslits or nanochannels [3,4]. The presence of the latter ones results in such effects as enhanced auxeticity in some directions, an appearance of auxetic properties in directions where these properties were not observed before, or even to disappearing of the auxeticity in known auxetic directions.

Acknowledgements

Part of the calculations was performed at the Poznań Supercomputing and Networking Center (PCSS).

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Reversibility of thickness change in nonwovens

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It has recently been shown that some nonwoven fabrics can exhibit an auxetic response in the thickness direction upon specific post-manufacture processing treatment of the fabric. We wish to report here a detailed examination of the reversibility of this auxetic response.

Auxetic response in these nonwovens was found to be fully reversible for strains below 3 percent. This increase in thickness on extension can be thought to result from a combination of reversible and irreversible processes. At small strains (1%, 2% and 3%) - deformation processes such as straightening of bent/crimped fibers, fiber rotations and straightening of buckled/tilted columns - are likely to be reversible due in large part to the interconnectivity of matrix fibers and fibers in columnar arrays which arise from the needle punching process. At strains larger than 3 percent, the same deformations may become irreversible. Additionally, slippage of fibers from contact points, disentanglement of fibers, formation of new entanglements, and fiber breakage are irreversible changes. At small strains, when only the reversible processes are dominant, the thickness can return to its original value even after multiple strain cycles. However, at larger strains, irreversible processes begin to dominate and the original thickness cannot be fully recovered after removal of load. Multiple cycles can cause further disentanglements resulting in even less thickness recovery at higher cycles for higher strain values (5% and 10%).

Anisotropic expansivity of flexible metal organic frameworks

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Metal-organic framework (MOF) materials are extended solid structures composed of metal cations, or clusters of metals, linked in three dimensions by polydentate organic ligands. Their potential for porosity is at the focus of intense interest at present for applications in fields that zeolites find use, such as gas separation (molecular sieving), shape-selective catalysis and ion exchange. MOFs have the advantage of tunable structures and properties by judicious choice of a vast range of organic ligands as well as metal cations from all parts of the Periodic Table. Another exceptional property of certain MOFs is their structural flexibility, which can involve atomic displacements of several Ångströms with the crystallinity of the network maintained, and often the connectivity. A famous MOF in this respect is the structure known as MIL-53, first described by the group of Férey in Versailles almost 15 years ago [1]: this is known for a variety of metals (Al, Cr, Fe, Ga, Sc, In) and is made up of inorganic chains of metal octahedra, cross-linked by bidentate terephthalate ligands to give diamond-shaped channels as shown in the figure below. The response of these materials to a variety of external stimuli is quite remarkable: with temperature, pressure, chemical modification or presence of extra-framework guest molecules, the material expands and contracts reversibly via a ‘wine-rack’ mechanism in a highly anisotropic fashion. I will present our own work on this material firstly by reviewing earlier results that show how the presence of solvent and/or guest molecules can be easily monitored using diffraction methods chemistry to define the flexible behaviour of the material [2]. Then I will show how we have been able to use chemical modification to induce unusual structural distortions of the structure in ways not seen before [3], or to tune the structural flexibility [4]. The relationship of these chemical modifications to thermal expansivity will also be explored with the aim of further understanding the underlying, atomic-scale mechanism of the structural flexibility.

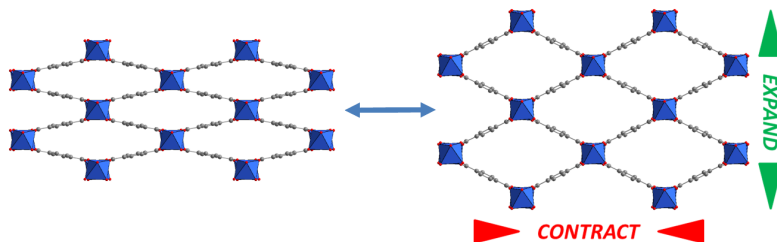


Figure 1. The reversible ‘wine-rack’ flexibility of the MIL-53 structure in response to external stimulus.

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Microstructural Effects on the Poisson's Ratio and Damping of Discs

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Isotropic and homogeneous solid materials may possess negative Poisson's ratio (ν) [1]. According to the theory of elasticity, the allowable range for Poisson's ratio in two-dimensional and three-dimensions solids are $-1 < \nu < 1$ and $-1 < \nu < 0.5$, respectively [2]. In this study, the finite element numerical method is adopted to calculate the effective Poisson's ratio and effective moduli of microstructured discs, as well as their linear viscoelastic damping. Fig. 1 shows the microstructured discs in terms of the auxetic angle (θ). When $\theta > 0$, the shape of the unit cell is reentrant, which is expected to exhibit effective negative Poisson's ratio.

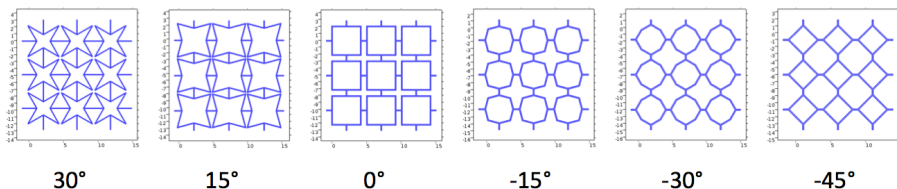


Figure 1. Microstructured discs with designated auxetic angle (θ). A zoom-in of $\theta = 30^\circ$ microstructure is shown in the inset of Figure 2 (a).

Purely elastic analysis of the microstructured discs with the plane strain assumptions indicates that their Poisson's ratio, effective bulk modulus (K_{eff}), effective Young's modulus (E_{eff}) and effective shear modulus (G_{eff}) are strongly dependent on the auxetic angle, as shown in Fig. 2 (a). When $\theta = 30^\circ$, the effective Poisson's ratio of the disc is -0.5, which leads to equal Young's modulus and shear modulus, according to isotropic elasticity. Maximum Poisson's ratio $\nu = 1$ is attained when $\theta = -45^\circ$. Assumed the solid phase behaves as a standard linear solid, the viscoelastic damping in terms of $\tan \delta$ at 1 Hz of the discs under uniaxial loading is shown in Fig. 2 (b), where the horizontal line is the calculated damping for 2D isotropic and homogeneous continuum for comparison. Due to the microstructural effects, the effective loss tangent of the discs reaches a minimum around $\theta = 20^\circ$. In addition, effects of plane stress assumptions, frequency, unit cell sizes and deformation amplitudes will be discussed.

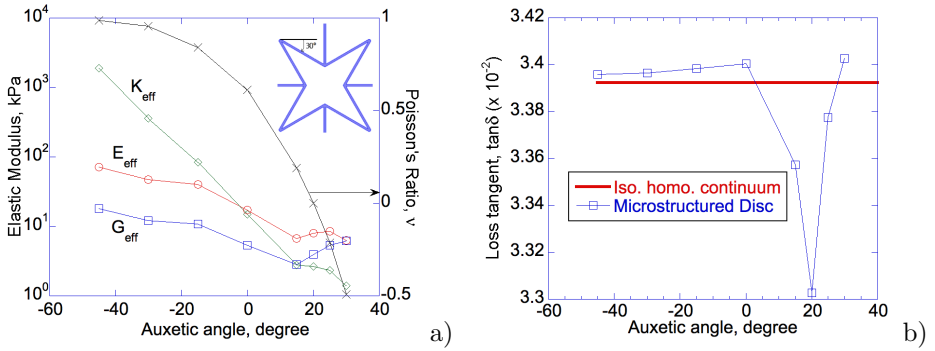


Figure 2. Effective bulk modulus, Young's modulus, shear modulus and Poisson's ratio, and b) effective loss tangent of the microstructured discs.

Acknowledgements

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Negative thermal expansion and other anomalous properties in metal fluorides with structures related to that of ReO_3

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Materials with a cubic- ReO_3 structure have long been suggested as good candidates for negative thermal expansion (NTE). Additionally, the simplicity of the cubic- ReO_3 structure is appealing for studies focused on understanding the factors governing a material's properties. In 2010, the first ReO_3 -type material to display strong NTE over a broad temperature range, ScF_3 , was reported. Subsequently, we have prepared and examined by variable temperature and pressure diffraction experiments the effects of solid solution formation in $\text{Sc}_{1-x}\text{M}_x\text{F}_3$ (M—trivalent cation), and the properties of the cation ordered ReO_3 -type ABF_6 (A—divalent ion, B tetravalent ion). This work revealed an array of unusual properties including very strong negative thermal expansion, pronounced elastic stiffening on heating, strong softening on compression and temperature dependent porosity.

Structural and mechanical properties of pentagraphene: preliminary molecular statics/molecular dynamics studies

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Pentagraphene is a new carbon allotrope the existence of which was proposed theoretically last year [1]. Its structure resembles the well-known Cairo tiling, forming a layer of pentagons constructed from a mixture of sp^2 - and sp^3 -coordinated carbon atoms.

We performed molecular statics simulations of structural and mechanical properties of pentagraphene. The obtained results have shown that – among all the tested empirical potentials – it is only the LCBOP [2] potential that is able to describe correctly the interactions in this carbon allotrope, reproducing the results of the *ab initio* calculations [1].

During the presentation the results of molecular dynamics simulations will be also presented, showing that pentagraphene reveals auxetic properties. The dependence of the mechanical properties on the temperature will be described and the mechanism of auxeticity will be explained.

Acknowledgements

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Simple models exhibiting negative Poisson's ratio

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Stretched materials change their shape and this change is described by Poisson's ratio, which is non-negative for common materials, like rubber, steel, etc. [1]. Stability conditions imply that for isotropic materials Poisson's ratio is a number between -1 and $1/(D - 1)$, where D is the dimensionality of the studied system [2]. Almost thirty years ago, foams with negative Poisson's ratio (NPR) have been manufactured [3]. The first mechanical model of Poisson's ratio equal -1 was proposed by Almgren [4] and the first thermodynamically stable NPR phase was the tilted (chiral) phase of hard cyclic-hexamers [5]. Since that time the interest in materials and models with NPR has grown and various mechanisms leading to this unusual effect have been described, see e.g. the recent book by Lim [6] and eleven focus issues of *Physica Status Solidi B*, to which references can be found in the last of them [7] and in references there in.

In this lecture some recent studies on selected mechanisms leading to NPR are reviewed briefly.

The hard cyclic hexamers studied in [5] were model molecules obtained by placing hard discs of equal diameters in vertices of perfect hexagons of the side lengths equal to the disc diameter. When the disc diameter is different from the hexagon side length one obtains hard cyclic hexamer molecules of any required anisotropy. By simple symmetry arguments one can show that they form a periodic structure at close packing (*zero temperature*) [8]. The hard hexamers can be thought of as the limit of the soft cyclic hexamers interacting through the n -inverse potential [8]. The static model of the latter particles can be solved exactly when the intermolecular interactions are reduced to the nearest-neighbouring 'atoms' [8]. (Further simplification of the intermolecular interactions in hexamers leads to the periodic hexachiral structure which was proposed in [9] and which exhibits the extreme Poisson's ratio equal -1 .) For *positive temperatures* the analytic methods fail both for hard and soft hexamers but structural and thermodynamic properties of these systems can be obtained by computer simulations. The properties of hard hexamers for the full range of anisotropy parameters are described in [10]. It is worth to stress that when the molecular anisotropy is sufficiently high, the Poisson's ratio can be arbitrarily close to -1 .

Obviously, the mechanism observed in planar hexamers is not the only one responsible for NPR at the microscopic level. Simple (planar or three-dimensional) examples studied recently are those with nano-channels [11,12], nano-slits [13], nano-layers [14], and other nano-inclusions [15].

As it follows from [16,17], both soft as well as rigid inclusions can lead to NPR also at the macroscopic level.

Acknowledgements

Part of the calculations, on which this work is based, was performed at the Poznań Supercomputing and Networking Center (PCSS).

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Auxeticity in a system of densely packed polymers

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The rules for auxetic properties of a system of polymers densely packed in a volume with an array of voids are discussed. To this aim a computer simulation approach was applied to describe the kinetics of reptating polymers subjected to mechanical stretching and/or compressing. The Poisson's ratio and isothermal compressibility were calculated for the system of polymers in the case of different shapes of the prepared voids.

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Piezo-morphic bone scaffold with auxetic behavior

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Bone healing and repair does not happen successfully without using a graft when the defects are large or in pathological fractures. When the bone or the surrounding tissues become infected or are not supplied with enough blood, bone healing can be negatively affected by causing delayed unions or non-unions. Maintaining a constant bone mass requires a correct balance between bone resorption and osteogenic function [1,2]. Different bone-grafts have extensively been used to overcome bone fracture occurred by diseases or injuries, however the mechanical properties of the bone still requires studies before designing and fabricating the bone graft and scaffold. A smooth transition from one shape to another as a consequence of environmental stimuli introduces a term of material called “morphic”. This terms has been identified by displaying stress-induced shape change due to gradient microstructure and elastic properties of material. Piezo-morphic also belongs to this category of term which shows responses to mechanical stimuli. Here, “morphic” means the ability to deform and undergo a smooth transition from one shape to another and “piezo” denotes the change of shape in response to a mechanical stress. Alderson et al (2013) exemplified piezo-morphic materials such as Polyurethane foam and microporous polymer (expanded polytetrafluoroethylene) [3]. This study tends to extend the above terms and introduces such a design and fabrication of a scaffold in which the ultimate structural and mechanical properties resemble either cortical or cancellous bone tissue (with changing the porosity and density in different directions). Scaffold fabricated based on this novel approach is expected to undergo shape changes (Piezo-morphic materials) while the mechanical load is applied and thus the influence of this shape change is of particular interest from the bone regenerative point of view. Mimicking visco-elastic properties of bone tissue may provide an environment for more favourable bone cells proliferation and growth and enhanced modelling and remodelling during the mechanical loading. The main challenge is to experience the fabrication technique which has been used for years but there has not been a single report for the fact that the fabricated scaffold with isotropic and anisotropic properties is useful for bone regeneration application.

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INDEX OF AUTHORS

A

Abaidia, C., 25
Airoldi, A., 11
Al-Badani, K., 36
Alderson, A., 42, 54, 75
Allen, T., 54
Astori, P., 11
Attard, D., 15, 20, 24
Azzopardi, K. M., 22

B

Bezazi, A., 25
Bilski, M., 13
Brańka, A. C., 27, 39, 40
Brincat, J. P., 22

C

Caruana-Gauci, R., 15, 19, 24
Cheng, H. C., 16
Cuierrier, É., 50
Czarnecki, C., 17

D

Daoudi, N., 25
Degabriele, E. P., 24
Dini, D., 27, 39, 40
Dobah, Y., 18
Dudek, K. K., 19, 20, 22, 24
Dudek, M. R., 19, 20, 22, 74
Duncan, O., 54
Dyskin, A. V., 21, 47, 60

E

Evans, K. E., 20

F

Farinelli, R., 11
Foster, L., 54
Fritzkowski, P., 43

G

Gatt, R., 19, 20, 22, 24
Gilardelli, A., 11
Godbole, P., 54
Goldstein, R. V., 23, 38
Gorodtsov, V. A., 23, 38
Grech, M. C., 24
Griffin, A. C., 65
Grima, J. N., 15, 18–20, 22, 24
Gu, Y., 36

H

Harkati, E., 25
Heyes, D. M., 27, 39, 40
Ho, D. T., 28
Hu, H., 29
Hyżorek, K., 32, 33

J

Jopek, H., 34
Jordan-Mahy, N., 54

K

Kadic, M., 35, 53
Kern, C., 35, 53
Kim, S. Y., 28
Kowalik, M., 45

L

Lake, M., 36
Le Maitre, C. L., 54
Lewiński, T., 17
Li, S. D., 36
Liao, S. M., 68
Lim, T. C., 37
Lisovenko, D. S., 23, 38

M

Maćkowiak, S., 39, 40

Mandhani, S., 42
Maruszewski, B. T., 43
Mizzi, L., 20, 24
Mott, P. H., 44

N

Narojczyk, J. W., 45, 48
Ng, W. S., 29
Novak, N., 46

P

Panichelli, P., 11
Pasternak, E., 21, 47, 60
Pieprzyk, S., 40
Pigłowski, P. M., 32, 48, 64
Porzio, F., 50
Poźniak, A. A., 51

Q

Qu, J., 53

R

Ren, J., 36
Ren, Z., 46
Roe, J., 54
Roh, J. H., 44
Roland, C. M., 44
Rushchitsky, J., 57
Rybicki, J., 71

S

Scarpa, F., 16, 18, 25
Shaheen, M. Y., 71
Shen, M. W., 68
Shofner, M. L., 65
Shufrin, I., 60
Soldera, A., 50
Stręk, T., 34, 61

T

To, M. K. B., 18
Tretiakov, K. V., 32, 33, 48, 64

U

Underhill, R. S., 50
ur Rehman, I., 42, 75

V

Verma, P., 65

Vesenjaj, M., 46
Volkov, M. A., 23

W

Walton, R. I., 66
Wang, Y. C., 68
Wegener, M., 35, 53
Wespiser, C., 50
Wilkinson, A. P., 70
Winczewski, S., 71
Wojciechowski, K. W., 13, 19, 32, 45,
48, 51, 64, 72
Wolak, W., 19, 74

Z

Zolgharnein, P., 42, 75