



Institute of Molecular Physics
Polish Academy of Sciences



Workshop on
Auxetics and related systems

June 27-30, 2004
Będlewo near Poznań, Poland

Programme and Abstracts

Poznań, 2004

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SPEAKERS

Alderson A. (Bolton, UK)
Alderson K. L. (Bolton, UK)
Dmitriev S. (Tokyo, Japan)
Gaspar N. (Exeter, UK)
Griffin A. C. (Atlanta, GA, USA)
Grima J. (Msida, Malta)
Heyes D. M. (Guildford, UK)
Hoover W. G. (Davis, CA, USA)
Idzikowski B. (Poznań, Poland)
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Schreiber J. (Dresden, Germany)
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Tokmakova S. P. (Moscow, Russia)
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Wei G. Y. (Beijing, China)
Wojciechowski K. W. (Poznań, Poland)

Programme of the Workshop *Auxetics and related systems*

27.06.2004 (Sunday)

8.30 leaving IFM PAN guest rooms (bus)

8.45 leaving GROMADA hotel (bus)

9.15 ÷ 9.45 visiting Poznań city centre

10.15 arrival to Kórnik

10.30 ÷ 11.45 visiting the Castle and the Library in Kórnik

11.45 ÷ 12.15 visiting the Arboretum in Kórnik

13.00 arrival to Będlewo

13.15 ÷ 14.15 lunch

14.30 ÷ 17.45 afternoon sessions

Chairman of the session: **Krzysztof Wojciechowski**

14.30 ÷ 14.45 **Opening**

14.45 ÷ 15.45 **Anselm Griffin (anselm.griffin@ptfe.gatech.edu)**

*Toward molecular auxetics: synthesis, structure, and
characterization of main chain liquid crystalline polymers
consisting of laterally attached para-quaterphenyls*

15.45 ÷ 16.15 coffee break

Chairman of the session: **Anselm Griffin**

16.15 ÷ 17.00 **Krzysztof Wojciechowski (kww@man.poznan.pl)**

Simple mechanisms leading to $\nu < 0$

17.00 ÷ 17.45 **Gaoyuan Wei (gywei@chem.pku.edu.cn)**

*Modelling of one, two and three dimensional molecular
auxetics*

18.00 welcome party (dinner)

28.06.2004 (Monday)

7.30 ÷ 8.45 breakfast

9.00 ÷ 12.45 morning sessions

Chairman of the session: **Fabrizio Scarpa**

9.00 ÷ 10.00 Andrew Alderson (a.alderson@bolton.ac.uk)
Modelling the deformation mechanisms, structure-property relationships and applications of auxetic nanomaterials

10.00 ÷ 10.45 Massimo Ruzzene (massimo.ruzzene@ae.gatech.edu)
Directional and band gap behaviour of periodic auxetic lattices

10.45 ÷ 11.15 coffee break

Chairman of the session: **Georgios Stavroulakis**

11.15 ÷ 12.00 Kim Alderson (k.alderson@bolton.ac.uk)
How to make auxetic fibre reinforced composites

12.00 ÷ 12.45 Naveen Ravirala (nr1res@bolton.ac.uk)
Expanding the range of auxetic polymeric products using a novel melt-spinning route

13.00 ÷ 13.45 lunch

14.00 ÷ 15.45 afternoon session

Chairman of the session: **Andrew Alderson**

14.00 ÷ 15.00 Georgios Stavroulakis (gestavr@cc.uoi.gr)
Auxetic behaviour: appearance and engineering applications

15.00 ÷ 15.45 Hajime Kimizuka (kimizuka.hajime@jri.co.jp)
Temperature elasticity of SiO₂ polymorphs: structural phase transition and elastic anomaly

15.45 ÷ 16.15 coffee break

16.15 ÷ 17.45 poster session

18.00 bonfire party

29.06.2004 (Tuesday)

7.30 ÷ 8.45 breakfast

9.00 ÷ 12.45 morning sessions

Chairman of the session: **David Heyes**

9.00 ÷ 10.00 William Hoover (hoover1@llnl.gov)
Searching for auxetics with DYNA3D and ParaDyn

10.00 ÷ 10.45 Joseph Grima (joseph.grima@um.edu.mt)
Auxetic behaviour from rotating rigid units

10.45 ÷ 11.15 coffee break

Chairman of the session: **Kim Alderson**

11.15 ÷ 12.00 Jürgen Schreiber (schreibe@eadq.izfp.fhg.de)
Thin Al-layers sputtered onto polyimide - an auxetic?

12.00 ÷ 12.45 Peter Švec (fyzisvec@savba.sk)
Al-based systems with unusual mechanical and transport properties

13.00 ÷ 13.45 lunch

14.00 ÷ 17.45 afternoon sessions

Chairman of the session: **William Hoover**

14.00 ÷ 15.00 David Heyes (d.heyes@surrey.ac.uk)
Liquids at negative pressure

15.00 ÷ 15.45 Jakob Schiøtz (schiotz@fysik.dtu.dk)
Atomic-scale modelling of plastic deformation of nanocrystalline copper

15.45 ÷ 16.15 coffee break

Chairman of the session: **Jürgen Schreiber**

16.15 ÷ 17.00 Toshiji Kanaya (kanaya@scl.kyoto-u.ac.jp)
Thermal expansion and contraction of polymer thin films

17.00 ÷ 17.45 Bogdan Idzikowski (idzi@ifmpan.poznan.pl)
Interface physics in nanocrystalline magnets

18.00 ÷ 19.00 round table discussion

19.00 banquet (dinner)

30.06.2004 (Wednesday)

7.30 ÷ 8.45 breakfast

9.00 ÷ 12.45 morning sessions

Chairman of the session: **Toshiji Kanaya**

9.00 ÷ 10.00 Fabrizio Scarpa (f.scarpa@shef.ac.uk)
Auxetic compliant flexible PU foams: static and dynamic properties

10.00 ÷ 10.45 Neil Gaspar (n.gaspar@physics.org)
Quantitative analysis of the microscale of auxetic foams

10.45 ÷ 11.15 coffee break

Chairman of the session: **Sergey Dmitrev**

11.15 ÷ 12.00 Jarosław Rybicki (ryba@task.gda.pl)
Molecular dynamics simulations of nanomechanical properties of metals

12.00 ÷ 12.45 Svetlana Tokmakowa (sveta@akin.ru)
Stereographic projections of Poisson's ratio in auxetic crystals

13.00 ÷ 13.45 lunch

14.00 ÷ 17.45 afternoon sessions

Chairman of the session: **Hajime Kimizuka**

14.00 ÷ 15.00 Sergey Dmitriev (sergey@iis.u-tokyo.ac.jp)
Discrete and continuum models for crystalline media with microscopic rotations

15.00 ÷ 15.45 Konstantin Tretiakov (kvt@ictp.trieste.it)
Monte Carlo simulations of hard body systems with extreme values of the Poisson ratio

15.45 ÷ 16.15 coffee break

Chairman of the session: **Jarosław Rybicki**

16.15 ÷ 16.45 Vitaly Novikov (novikov@te.net.ua)
Extreme viscoelastic properties of composites of fractal structures due to negative stiffness phases

16.45 ÷ 17.00 Closing

18.00 ÷ 19.00 dinner

19.30 leaving Będlewo (return to GROMADA hotel in Poznań)

Preface

Modern technology requires new materials of special properties. One of reasons for interest in materials of unusual mechanical properties comes from the fact that they can be used as matrices to form composites with other materials of other required properties: electric, magnetic, etc.

A new field of endeavour are studies of materials exhibiting anomalous (negative) Poisson's ratio, first manufactured in 1987 (by R. S. Lakes) and later coined (by K. E. Evans) *auxetics*, which, in contrast to typical materials (like rubber, glass, metals, etc.), expand transversely when pulled longitudinally and contract transversely when pushed longitudinally. This counterintuitive property is essential from the point of view of modern technology - many applications of the auxetics have been designed in various fields of human's activity, from vascular implants, strain sensors, shock and sound absorbers, "press-fit" fasteners, gaskets, air filters,...to fillings for highway joints.

Materials containing inclusions of negative stiffness constitute another class of systems with unusual mechanical properties. The recent interest in such systems has its origin in their very high damping.

Systems of extreme hardness, composites of hierarchical structures, polymers of negative thermal expansivity and other materials of anomalous mechanical properties, having a lot of potential applications, are also within the reach of the methods of modern science.

Analytical, computer, and experimental studies and modelling of such systems

- a) offer *better understanding* of known mechanisms responsible for their unusual properties and
- b) suggest *new mechanisms* which may lead to obtaining new materials of required features.

Thus, investigations of the above non-conventional systems are interesting and important both from the point of view of fundamental research and from the point of view of possible practical applications.

The following topics, essential to the physics of auxetic and related materials, are within the scope of the Workshop:

1. properties and applications of auxetic materials,
2. mechanisms leading to auxetic behaviour,
3. experimental studies of auxetic materials,
4. multifunctional systems incorporating auxetic behaviour,
5. systems of special mechanical properties (e.g. systems with inclusions of negative stiffness, composites of hierarchical structures, systems of extreme hardness, etc.),
6. theoretical and computer simulation methods for modelling auxetics and other systems of special mechanical properties.

The main objective of the Workshop is to gather scientists (experimentalists and theoreticians) from various in one place to exchange information on new experimental and theoretical results and methods in the field of materials of unusual mechanical (elastic and/or visco-elastic) properties (materials of negative

Poisson's ratio, materials with negative stiffness inclusions, systems of extreme hardness, etc). The Workshop is also addressed to young scientists (students, Ph.D. students and post-docs), with the aim of acquainting them with theoretical, experimental and simulation methods used in the physics of such systems.

We hope that exchange of information and ideas will not only lead to better understanding and exploiting of the already known systems but also to formulation of directions for new research activities which, in turn, will lead to discovering and/or manufacturing of new 'anomalous' systems. The latter should attract a new generation of researchers to this fascinating field.

Krzysztof Wojciechowski

LECTURES

MODELLING THE DEFORMATION MECHANISMS, STRUCTURE-PROPERTY RELATIONSHIPS AND APPLICATIONS OF AUXETIC NANOMATERIALS

A. Alderson¹, K. L. Alderson¹, K. E. Evans², J. N. Grima³, M. Williams¹,
P. J. Davies¹

¹ *Centre for Materials Research and Innovation, Bolton Institute, Bolton, UK*

² *Department of Engineering, University of Exeter, Exeter, UK*

³ *Department of Chemistry, University of Malta, Msida, Malta*

Negative Poisson's ratio materials undergo lateral expansion upon longitudinal tensile loading, and also lateral contraction under longitudinal compression, so-called *auxetic* behaviour. Other 'negative' materials include those displaying negative thermal expansion, negative permeability, negative permittivity and negative refractive index properties. Negative materials are currently attracting much interest due to their counter-intuitive behaviour and also in applications where the negative property itself, or enhancements in other materials properties due to the negative property, may be exploited. In all cases the unusual properties are related to the structure of the materials, leading to a need to develop increased understanding of the mechanisms acting within the material from the molecular to macro scales. For example, natural and synthetic auxetic materials and structures are known due to deformation mechanisms acting at the nano- to the micro- and macroscopic levels.

The discovery in 1992 that the α -cristobalite polymorph of crystalline silica possesses negative Poisson's ratios has led to an increase in research into the modelling, design and development of auxetic nanomaterials. Nanoauxetics are, in particular, expected to have potential in sensor, molecular sieve and separation technologies, as well as providing a route to high modulus auxetic materials for structural applications.

This paper will briefly review some of the early attempts at designing and modelling auxetic behaviour at the nanoscale and will report results from our more recent modelling investigations into the structures, deformation mechanisms, mechanical and mass transport properties of a range of auxetic nanomaterials. In particular, analytical expressions for the Poisson's ratios of certain crystalline silica polymorphs have been developed which reproduce the experimental values for loading in the x_3 direction remarkably well, explaining in the process the dichotomy between negative and positive values of Poisson's ratio in α -cristobalite and α -quartz, respectively. The analytical models have been extended to: investigate strain dependency of the Poisson's ratio; predict uniaxial stress-induced second phases; and have also been applied to the germania analogues of α -cristobalite and α -quartz.

Molecular mechanics simulations of silica and a number of idealised zeolite cage structures, which are predicted to be auxetic, will also be reported. Results from Monte Carlo simulations for the strain-dependent sorption of molecules onto

the MFI (ZSM5 – Si₉₆O₁₉₂) zeolite all-silica structure demonstrate the potential for using auxetic nanomaterials in tunable and selective sieving and switching devices, and in, for example, drug and gene delivery.

Finally, the possible link between negative Poisson's ratio and negative thermal expansion coefficient behaviour has been investigated using analytical methods. It is suggested that the preliminary results indicate such a link may be realisable at the nanoscale.

HOW TO MAKE AUXETIC FIBRE REINFORCED COMPOSITES

K. L. Alderson¹, V. R. Simkins¹, V. L. Coenen¹, P. J. Davies¹, A. Alderson¹
and K. E. Evans²

¹ *Centre for Materials Research and Innovation, Deane Road, Bolton, BL3 5AB, UK*

² *Department of Engineering, Computer Science and Mathematics, University of Exeter,
North Park Avenue, Exeter EX4 4QF, UK.*

Developments in structural engineering design and technology over the past three decades in industries such as aircraft, automobile and sports and leisure equipment have demanded the production of new, high-performance materials. Within this class of materials are the fibre-reinforced composites. Advances in auxetic materials production and development have led to the possibility of producing auxetic fibre reinforced composites, thus exploiting property enhancements known to arise in auxetic materials such as energy absorption, improved fracture toughness and better resistance to indentation.

There are a number of ways in which auxetic fibre reinforced composites can be made. The route closest to conventional manufacture is to use off-the-shelf prepreg material which, given specific stacking sequences, will produce an overall auxetic effect. Several groups have used this route to auxetic fibre reinforced composites [1-5] and have made some inroads into testing the resultant materials for enhanced fracture toughness [3] and indentation resistance [4]. Work recently carried out in Bolton has studied the static indentation and low velocity impact resistance of auxetic carbon fibre laminates and has found some interesting results in terms of localisation of damage and enhancements in energy absorption in particular, which will be discussed here.

A further method of manufacturing an auxetic fibre reinforced composite is to use auxetic components, for example, an auxetic matrix, auxetic reinforcement or both. This has been achieved using auxetic foams previously [6] and has been modelled for some considerable time [7]. However, it has only very recently been possible to begin work on auxetic fibre reinforced composites of this type with the advances in the manufacture of auxetic fibres and new methods to produce auxetic polymers. Current work at Bolton is assessing the possibility of using auxetic polymeric fibres within a composite. The fibres used to date are polypropylene and tests have been carried out to assess their pull-out performance from a specially designed matrix. The results have shown that it is up to 4 times more difficult to pull out an auxetic fibre than a similar conventional fibre. The results and their implications will be discussed, together with ongoing work to deploy these fibres within a composite material for low velocity impact testing and mechanical property assessment.

References

[1] C. T. Herakovich, *Comp. Mater.* **18**, 447 (1984).

- [2] J. F. Clarke, R. A. Duckett, P. J. Hine, I. J. Hutchinson, and I. M. Ward, *Composites* **25(9)**, 863 (1994).
- [3] J. Chandhur and Q Jang, Proc. Am. Soc. Compos. 3rd tech conf, Seattle WA, Sept. 25-29 1988, Ed. J. C. Serais, J. T. Quilow, Tech. Pub. Co. Inc. pp701.
- [4] J. P. Donoghue, PhD Thesis, University of Liverpool, 1992.
- [5] R. Zhang, H. L. Yeh, and H. Y. Yeh, *J. Reinf. Plast. and Comp.* **17(18)**, 1651 (1982).
- [6] R. S. Lakes and C. P. Chen, *J. Mat. Sci.* **28**, 4288 (1993).
- [7] M. J. Nkansah, K. E. Evans, and I. J. Hutchinson, *J. Mat. Sci.* **28**, 2687 (1993).

DISCRETE AND CONTINUUM MODELS FOR CRYSTALLINE MEDIA WITH MICROSCOPIC ROTATIONS

S. V. Dmitriev¹, A. A. Vasiliev², N. Yoshikawa¹, T. Shigenari³,
Y. Ishibashi⁴

¹ *Institute of Industrial Science, The University of Tokyo, Japan*

² *Department of Mathematical Modeling, Tver State University, Tver, Russia*

³ *Department of Applied Physics and Chemistry, The University of Electro-Communications, Tokyo, Japan*

⁴ *Faculty of Communications, Aichi Shukutoku University, Aichi Prefecture, Japan*

Microscopic rotations can play a very important role in the molecular crystals or in some dielectric crystals where atoms are joined in comparatively rigid clusters and the inter-cluster interactions are comparatively weak. The range of unusual phenomena observed in such materials is fascinating, from incommensurate phase to negative Poisson ratio. Here we discuss these and other phenomena in frame of the 1D and 2D elastically hinged molecule (EHM) models having microscopic particles with rotational degrees of freedom.

We also discuss the topological soliton dynamics in such materials and describe a number of effects, such as the trigger off and propagation of auto-waves, soliton multiplication in the metastable media, soliton collisions and annihilations.

For this model we construct various continuum approximations. New important features of the continuum models for media with microscopic rotations are the increase in number of equations of motion due to the increase in number of degrees of freedom and the appearance of the higher gradient terms in the resulting equations. We also construct the multi-field (MF) continuum approximation capable of description not only long but also short waves. The later feature of the MF theory is very important for the materials having finite size particles because for them a strong coupling of long and short waves takes place very often. MF continuum theory can be constructed for a discrete system considering *more than one* primitive translational cell. As for the discrete system, consideration of elementary volume with more than one primitive cell adds no new physical details. However, continuum analog for the discrete system with extra degrees of freedom is valid for both long and short waves, see, e.g., A. A. Vasiliev, *Moscow Univ. Mech. Bull.* **51**, 44 (1996).

QUANTITATIVE ANALYSIS OF THE MICROSCALE OF AUXETIC FOAMS

N. Gaspar¹, C. W. Smith¹, G. Seidler², and K. E. Evans¹

¹ *School of Engineering, Computer Science and Mathematics, Harrison Building, North Park Road, University of Exeter, Exeter, Devon EX4 4QF, UK.*

² *Department of Physics, Box 351560, University of Washington, Seattle, WA 98195-1560, USA*

The auxetic foams first produced by Lakes have been modelled in a variety of ways, each model trying to reproduce some observed feature of the microscale of the foams. Such features include bent or broken ribs or inverted angles between ribs. These models can reproduce the Poisson's ratio or Poisson's function of auxetic foam if the model parameters are carefully chosen. However these model parameters may not actually reflect the internal structure of the foams. A big problem is measurement of parameters such as lengths and angles is not straightforward within a 3-d sample. In this work a sample of auxetic foam has been imaged by 3-d x-ray computed tomography. The resulting image is translated to a form that emphasises the geometrical structure of connected ribs. This connected rib data is suitably analysed to describe both the microstructural construction of auxetic foams and the statistical spread of structure that is the heterogeneity of an auxetic foam. From the analysis of the microstructure, observations are made about the requirements for microstructural models and comparisons made to the model parameters of previous existing models. From the statistical data, measures of heterogeneity are made that will help with future modelling that includes the heterogeneous aspect of auxetic foams.

TOWARD MOLECULAR AUXETICS: SYNTHESIS, STRUCTURE, AND CHARACTERIZATION OF MAIN CHAIN LIQUID CRYSTALLINE POLYMERS CONSISTING OF LATERALLY ATTACHED PARA-QUATERPHENYLS

C. He^{1,2}, P. Liu¹ and A. C. Griffin^{1,2*}

¹ *Departments of Chemistry & Biochemistry, University of Southern Mississippi, Hattiesburg, MS 39406 USA*

² *Departments of Polymer Science University of Southern Mississippi, Hattiesburg, MS 39406 USA*

Polymers containing para-quaterphenyl rods laterally attached to the polymer main chain have been synthesized. The molecular design choices which led to use of the quaterphenyl rod to achieve auxetic response will be discussed. Preparative chemistry of the monomers will be described along with the details of the polymerization reaction. Both polyethers and polyesters were prepared. The length of the flexible alkyl main chains which link the rods plays an important role in determining whether the resulting polymers will exhibit liquid crystallinity. Thermal and optical data will be presented in support of liquid crystallinity of these polymers. Polymers with longer alkyl linkages exhibit nematic liquid crystallinity and the rods appear to have their long axes oriented roughly parallel and along the main chain direction.

X-ray scattering experiments were performed on the polymers both in the quiescent (unstretched) and the stretched states. Results from these experiments suggest that, under tensile strain, site connectivity driven rod-reorientation occurs in these materials giving rise to an increase in the interchain distance for these polymers. This increase in the interchain separation is consistent with our concept of a molecular level auxetic mechanism for this type of designed polymer.

We would like to thank the U.S. Air Force of Scientific Research (F49620-1-0078) for financial support of this work. We also wish to thank the National Science Foundation for thermal instrumentation facilities (DMR-95112506).

* Current address: School of Polymer, Textile, and Fiber Engineering; Georgia Institute of Technology, Atlanta GA 30332 USA

AUXETIC BEHAVIOUR FROM ROTATING RIGID UNITS

J. N. Grima¹ and K. E. Evans²

¹ *Department of Chemistry, University of Malta, Msida MSD 06, MALTA.*

² *Department of Engineering, University of Exeter, Exeter, UK.*

Auxetic materials exhibit the unexpected feature of becoming fatter when stretched and narrower when compressed, in other words, they exhibit a negative Poisson's ratio. This counter-intuitive behaviour imparts many beneficial effects on the material's macroscopic properties that make auxetics superior to conventional materials in many commercial applications.

Recent research suggests that auxetic behaviour generally results from a synergism between the material's internal structure (geometry setup) and the deformation mechanism it undergoes when submitted to a stress. This means that auxetic behaviour is scale-independent, and thus, the same geometry/deformation mechanism may operate at the macro-, micro- and nano- (molecular) level. Historically, a considerable amount of research has been focused on the 're-entrant honeycomb structure' which exhibits auxetic behaviour if deformed through hinging at the joints of flexure or the ribs, and it was proposed that this 're-entrant' geometry plays an important role in generating auxetic behaviour in various forms of materials ranging from nanostructured polymers to foams.

This paper discusses an alternative mode of deformation involving 'rotating rigid units' which also results in negative Poisson's ratios. In its most ideal form, this mechanism may be constructed in two dimensions using 'rigid polygons' connected together through hinges at their vertices. On application of uniaxial loads, these 'rigid polygons' rotate with respect to each other to form a more open structure hence giving rise to a negative Poisson's ratio. More generally, this mechanism may be constructed using rigid three dimensional rigid units such as tetrahedra, cuboids, *etc.* This paper also discusses the role that 'rotating rigid units' are thought to have in various classes of materials to give rise to negative Poisson's ratios.

LIQUIDS AT NEGATIVE PRESSURE

D. M. Heyes¹, C. Xiao¹, and J. G. Powles²

¹ *Division of Chemistry, School of Biomedical & Molecular Sciences, University of Surrey,
Guildford GU2 7XH, United Kingdom,*

² *Centre for Complex Fluid Processing, School of Engineering, University of Wales
Swansea, Singleton Park, Swansea SA2 8PP*

Auxetic materials have the distinctive property that they dilate when subjected to uniaxial extension. While there are some naturally occurring solids that are auxetic, it is not clear yet whether there are any auxetic liquids. However, it is well-known that liquids *do* dilate when subjected to a *uniform* or isotropic tension (or ‘negative pressure’). These are metastable states however and the dilation only lasts for a short time before the liquid eventually releases the stress, usually by forming cavities, a phenomenon known as ‘cavitation’. It is a distinguishing feature of liquids that they can only support a shear stress over a finite period, and the situation is much the same for uniform tension. No liquid can be thermodynamically stable at a negative pressure.

In this talk I will give a summary of the field of ‘stretched liquids’ using experimental results and theory, and discuss the factors that govern cavity or ‘bubble’ formation. The most successful theoretical description of bubble formation is called Classical Nucleation Theory, CNT. This assumes equilibrium thermodynamics can be applied in the metastable negative pressure liquid region of the phase diagram, and is based on the fact that bubble formation is an activated process. Its predictions are remarkably accurate, and despite the simplicity of its formulae, this treatment has stood the test of time. CNT provides a relatively quick way of mapping out the general thermodynamic features of cavitation over the liquid-vapour region of the phase diagram, although to date it has been limited to relatively simple equations of state (EoS). We have extended CNT to include the more realistic van der Waals EoS [1]. We have derived analytic expressions for the vapour pressure inside the cavity, the equilibrium liquid/vapour, and spinodal volumes and pressures. The maximum tensile strength of water using this model, estimated from the liquid spinodal pressure close to the triple point, is *ca.* 800 bar which is within the error bounds of recent experiments. We also considered the Lennard-Jones fluid, as a representative ‘realistic’ fluid, using a literature-parameterised equation of state. This gives a slightly smaller value of *ca.* 600 bar for the maximum tensile strength of water near the triple point.

The collapse of a bubble in the liquid is of considerable importance in a number of fields, which has traditionally been modelled using a continuum hydrodynamics approach. When the bubble is in the final stages of its collapse, it has a diameter in the nanometer range, and it is more realistic to adopt a fully molecular description of the system, using either statistical mechanics [2] or Molecular Dynamics computer simulations [3]. I will show the results of Molecular Dynamics simulations of a collapsing bubble or cavity in a simple ‘Lennard-Jones’

liquid. A series of MD simulations was carried out with periodic boundary conditions using a cubic box containing up to 108,000 Lennard-Jones (LJ) particles to create initially an equilibrium bulk liquid. The evolution of the collapsing bubble, which we call a ‘Collapse Event’ (CE), was followed typically for a 1000 times starting from a statistically independent liquid configuration each time to improve the statistics of the (averaged) radial profiles. Radial density, normal pressure and temperature profiles were computed from the centre of the original cavity.

References

- [1] C. Xiao and D.M. Heyes, *Cavitation in Stretched Liquids*, Proc. Roy. Soc. Lond. A **458**, 889 (2002).
- [2] G. Rickayzen, and J. G. Powles, *A collapsing bubble in a fluid: a statistical mechanical approach*, Molecular Physics **100**, 3823 (2002).
- [3] C. Xiao, D. M. Heyes, and J. G. Powles, *The collapsing bubble in a liquid by molecular dynamics simulations*, Molecular Physics **100**, 3451 (2002).

SEARCHING FOR AUXETICS WITH DYNA3D AND PARADYN

W. G. Hoover and C. Hoover

University of California at Davis and Lawrence Livermore National Laboratory, Davis, CA, USA

We seek to simulate auxetic behavior by dynamic analyses of mesoscopic models. We generate nearly periodic cellular structures. "Shell" elements are the basic building block. The shells obey standard continuum mechanics. The dynamical response of the structures is then determined for a three-stage loading process: (1) homogeneous compression; (2) relaxation; (3) uniaxial compression. The simulations are carried out with both serial and parallel computer codes – DYNA3D and ParaDyn – which describe the deformation of the shells with an elastic-plastic equation of state and a robust contact algorithm.

INTERFACE PHYSICS IN NANOCRYSTALLINE MAGNETS

B. Idzikowski

*Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, 60-179
Poznań, Poland*

A comprehensive review of our recent experimental and theoretical developments in the processing of nanocrystalline soft magnetic materials made by crystallization of amorphous precursors and containing new nanocrystalline phases will be given. The relationship between the structures of the metastable and equilibrium phases and their transformations are discussed. The conditions of the phases formations are found to depend on the difference between the symmetries of equilibrium and metastable phases.

In soft magnetic nanocrystalline materials the effect of large anisotropy constant of crystalline phase could be highly suppressed by reducing the grain size to nanometer scales. Due to the magnetic exchange interactions nanocrystalline alloys consisting of magnetic grains placed in amorphous matrix can reveal a smooth magnetization curve with extremely small values of coercivity. This approach has been applied earlier to the development of FINMET, NANOPERM and HITPERM alloys and then also for new compositions of iron-nickel-based and iron-cobalt-based amorphous alloys. In such materials annealing favours the emergence of cubic $\text{Fe}_x(\text{Ni},\text{Co})_{23-x}\text{B}_6$ crystalline grains of several nanometers in diameter, as it was identified by XRD and transmission electron microscopy (TEM) measurements [1].

The Mössbauer spectrometry as a principal local technique to study the structure relation to magnetic behaviour of nanocrystalline alloys could be employed. In particular, the structural arrangement of nanograins, the role of grains shape, morphology of the grains surfaces, the magnetic interactions between them as well as ribbons surface properties studied by conventional and conversion electron Mössbauer spectrometry (CEMS) will be reported.

Final conclusions of the investigations were supported by supplementary information from differential scanning calorimetry, magnetostriction measurements, transmission electron microscopy and high resolution TEM.

The magnetic measurements were also supported by the calculations of Fe and Ni or Co magnetic moments in Fe_{23}B_6 and $\text{Fe}_{22}(\text{Ni},\text{Co})\text{B}_6$ phases using the spin polarized tight binding linear muffin-tin orbital (TB-LMTO) method. Band structure calculations showed that the local magnetic moments of Fe, Ni and Co atoms in Fe_{23}B_6 , Ni_{23}B_6 and Co_{23}B_6 compounds depend on their local environments (e.g. the iron magnetic moments are enhanced up to about $3 \mu_B/\text{atom}$). In particular, the calculations show that the Ni or Co impurities prefer the 4a and 48h site, respectively.

References

- [1] B. Idzikowski, J. M. Greneche, A. Szajek, and J. Kovač; Appl. Phys. Lett. (2004), in print.

THERMAL EXPANSION AND CONTRACTION OF POLYMER THIN FILMS

T. Kanaya

Institute for Chemical Research, Kyoto University, Uji, Kyoto-fu 611-0011, Japan

Properties of polymer thin films and/or polymer surfaces are very different from those of the bulk and related to many phenomena such as adhesion, wetting and surface friction. One of the most interesting but unusual phenomena observed in thin glassy polymer films is negative expansivity, which was first reported about 10 years ago.

In this work, we have studied thermal expansion and contraction of polymer thin films supported on Si substrate below and above the glass transition temperature to elucidate the origin of the negative expansivity. We found that apparent negative expansivity in glassy thin films disappeared for well-annealed thin films, suggesting that it is caused by the unrelaxed structure due to lack of annealing. We also found that even for long annealing the thermal expansivity of thin films below about 20 nm in glassy state is smaller than that expected from the bulk and almost zero below several nm. We will discuss the origin of the decrease in expansivity with film thickness based on the quasielastic neutron scattering data.

In addition, we also found an extremely slow contraction (annealing) process of thin films in the melt, which has relaxation time of about 30 - 50 h at 423 K, and furthermore an ultra-slow re-expansion process in the glassy state. In the meeting we will also discuss the origin of the ultra-slow contraction and re-expansion processes.

MOLECULAR DYNAMICS STUDY OF THE HIGH-TEMPERATURE ELASTICITY OF SiO_2 POLYMORPHS: STRUCTURAL PHASE TRANSITION AND ELASTIC ANOMALY

H. Kimizuka

Energy & Environment Technology Group, Science Division, The Japan Research Institute, Limited, 1-4-17 Misaki-cho, Chiyoda-ku, Tokyo, 101-0061, Japan

The elastic properties of quartz and cristobalite, the typical polymorphs of silicon dioxide (SiO_2), are studied with particular emphasis on the structural phase transition and the high-temperature phase. Using the equilibrium molecular dynamics method with the stress fluctuation formalism, I have successfully evaluated the adiabatic elastic constants (C_{ij}) of both quartz and cristobalite over the α - β phase transition. It is noteworthy that the calculated C_{ij} values of quartz are in good agreement with experiment in the entire temperature range of 300-1100 K, including the transition region. In the results of quartz, anomalous properties of a negative Poisson's ratio appear in the narrow temperature region between 750 and 800K before the phase transition occurs, where the bulk modulus is extremely low compared with the shear modulus. Here, quartz is susceptible to volumetric or bulk deformation, but is resistant to shear deformation. After the transition, the bulk modulus is shown to increase sharply, and a positive value of Poisson ratio is recovered due to the increase of thermal motions. I have confirmed that the net increase of bulk C_{ij} 's in the β phase can be attributed to the internal relaxations, which arise from the cooperative motions of corner-linked SiO_4 tetrahedra. These MD simulations have revealed the existence of dynamical disorder in β quartz at high temperatures, and its influence on the macroscopic elastic properties, in contrast to the ordered β -quartz structure model [1].

On the other hand, cristobalite exhibits a negative Poisson's ratio over the wide temperature range of 300-1800 K. I have found that the mechanisms differ between α and β phases from the atomistic motions of the molecular dynamics results. The SiO_4 tetrahedral framework structures of both phases are confirmed to be composed of flexible microcellular clusters with an inverted characteristic similar to re-entrant foams. A negative Poisson ratio arises from the folding or unfolding of these wells along the different directions in each phase [2-3].

References

- [1] H. Kimizuka, H. Kaburaki, and Y. Kogure, Phys. Rev. B **67**, 024105 (2003).
- [2] H. Kimizuka, H. Kaburaki, and Y. Kogure, Phys. Rev. Lett. **84**, 5548 (2000).
- [3] H. Kimizuka *et al.*, Prog. Theor. Phys. Suppl. **138**, 229 (2000).

EXTREME VISCOELASTIC PROPERTIES OF COMPOSITES OF FRACTAL STRUCTURES DUE TO NEGATIVE STIFFNESS PHASES

V. V. Novikov¹ and K. W. Wojciechowski²

¹ *Odessa National Polytechnical University, 1 Shevchenko Prospekt, 65044 Odessa, Ukraine*

² *Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, 60-179 Poznań, Poland*

The hierarchic model of structure [1] is generalized and applied to study viscoelastic properties of a two-component inhomogeneous medium with chaotic, fractal structure and with one of the components exhibiting a negative shear modulus. It is shown that similarly to the results obtained recently in frames of the Hashin-Strikman model [2], the present model predicts possibility to obtain composites of the effective shear and dumping coefficient much higher than those characterizing both the component phases. The viscoelastic properties of the fractal medium are, however, qualitatively different from the properties of the Hashin-Strikman medium [3].

References

- [1] V. V. Novikov, K. W. Wojciechowski, D. V. Belov, and V. P. Privalko, *Phys. Rev. E* **63**, 036120 (2001).
- [2] R. S. Lakes, *Phys. Rev. Lett.* **86**, 2897 (2001).
- [3] V. V. Novikov, K. W. Wojciechowski, in preparation.

EXPANDING THE RANGE OF AUXETIC POLYMERIC PRODUCTS USING A NOVEL MELT-SPINNING ROUTE

N. Ravirala, A. Alderson, K. L. Alderson, P.J. Davies

Centre for Materials Research and Innovation, Bolton Institute, Bolton BL3 5AB

The first auxetic fibre was successfully produced in polypropylene using a novel melt-spinning route. The auxetic fibres were extruded at 159°C with a screw speed 1.05 rads⁻¹ and 0.03 ms⁻¹ take-up speed. Characterisation of the fibres involved optical techniques (videoextensometry) to measure the strains along both the length and the width simultaneously during deformation.

The unique processing route has now been developed to expand the range of auxetic extruded polymeric products. We report here auxetic polypropylene films have been developed, and auxetic polyester and polyamide fibres have now been produced.

Recent theoretical investigations into the structures and mechanisms leading to auxetic behaviour in these products will be reported.

Finally, a review of some potential applications for auxetic fibres and films will be presented. These include as reinforcements in composites, anchoring devices, smart bandages for healthcare, breathable packaging and tear resistant films.

DIRECTIONAL AND BAND GAP BEHAVIOUR OF PERIODIC AUXETIC LATTICES

M. Ruzzene

School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA

The paper investigates the wave propagation characteristics of two-dimensional (2D), auxetic lattice structures. Periodic structures in general feature unique wave propagation characteristics, whereby waves are allowed to propagate only in specific frequency bands. Two-dimensional periodic structures complement this feature with a low frequency directional behavior. The combination of these unique characteristics makes two-dimensional periodic structures ideal candidates for the design of pass-band directional mechanical filters.

Focus is here placed on honeycomb lattice configurations. A sensitivity analysis is first presented to investigate the influence of band gap and directional behaviors with respect to changes in the internal angle. The presented results demonstrate how re-entrant topologies feature enhanced wave attenuation capabilities with respect to hexagonal lay outs. An optimization problem is then formulated by considering the internal angle as a design variable, and where the width of the attenuation zones and angular range of propagation at low frequencies are the objective functions. The identified optimal configurations show the combined properties of the considered assembly and the effectiveness of the analysis procedure.

Keywords: Two-dimensional periodic structures, auxetic periodic lattice, band gaps, directionality, optimization.

MOLECULAR DYNAMICS SIMULATIONS OF NANOMECHANICAL PROPERTIES OF METALS

J. Rybicki

*Department of Solid State Physics, Faculty of Technical Physics and Applied Mathematics
Gdansk University of Technology, Narutowicza 11/12, 80-952 Gdansk, Poland*

and

TASK Computer Centre, Narutowicza 11/12, 80-952 Gdansk, Poland

Working objects to obtain desired shapes and surface properties by removing layers of material with bladed tools is one of the most important technological processes. In technical sciences (and arts), methods are developed on the macroscopic level, usually with no reference to the atomic structure of matter. In the last twenty years, techniques of working materials with nanometric precision have been developed (instruments at Lawrence Livermore National Laboratories and Cranfield Unit for Precision Engineering). At the moment, there is still very few (very expensive) nanometric working devices of the required precision in guiding the tool, sufficient vibration damping and capable of keeping the necessary cleanliness of the worked surface. However, even using the best equipment does not guarantee full repeatability of experimental conditions and measurement results. Therefore, there is wide room for theoretical considerations, including atomistic molecular dynamics simulations.

The paper covers the latest achievements in the area of classical molecular dynamics simulations of nanomechanical properties of metals. It also includes a presentation of a *nanoMD* code currently developed at the Faculty of Technical Physics and Applied Mathematics of the Gdansk University of Technology.

The work has been sponsored by KBN, grant number 7 T11F 013 21. The calculations have been performed at the TASK Computer Centre, Gdansk. Poland.

AUXETIC COMPLIANT FLEXIBLE PU FOAMS: STATIC AND DYNAMIC PROPERTIES

F. Scarpa¹, P. Pastorino¹, A. Garelli¹ and S. Patsias²

¹ *Multidomain Cellular Solids Laboratory, Department of Mechanical Engineering
University of Sheffield, S1 3JD Sheffield, UK*

² *Department of Mechanical Engineering, University of Sheffield, S1 3JD Sheffield, UK*

Flexible polyurethane auxetic foams have been manufactured from conventional PU base cellular material with manufacturing process parameter different from [1] and [2]. The samples obtained are cylindrical, with the auxetic effect obtained varying longitudinal and radial compressions in function of temperature distribution during process. The foams have been subjected to quasi static tensile and compression tests at room temperature using tensometer and MTS 2050 machines. To acquire a comparison with current foams, conventional samples (used as starting base) and equivalent non-auxetic foam with the same density of the auxetic one [3] (and same core material for the cell struts) have been produced and tested.

The stress-strain curve of the compliant auxetic foams shows a significant difference from the conventional base used for manufacturing, with notably the absence of a distinct plateau stress region in compression, while the tensile elongation allows a failure strain around 120 %. Compared to the non-auxetic iso-density ones, the negative Poisson's ratio foams have an increase of around 25 % of the densification strains. Constant strain rate tests up to 30s-1 show also that the stress-strain curves for the auxetic foams are almost insensitive to the strain rate applied.

The auxetic and non-auxetic foams have been also tested under sinusoidal cycling load up to 10 Hz, with maximum pre-strain applied of 12 %. The hysteresis of the cycling loading curve has been measured to determine the damping hysteretic loss factor for the various foams. The measurements indicate that auxetic foam have an increased damping loss factor of 20 % compared to the non-auxetic foams. The energy dissipation is particularly relevant in the tensile segment of the curve, with effects given by the pre-strain level imposed on the samples.

References

- [1] N. Chan and K. E. Evans, *Fabrication methods for auxetic foams*. Journal of Material Science **32**, 5945 (1997).
- [2] F. Scarpa, L. G. Ciffo and J. R. Yates. *Dynamic properties of high structural integrity auxetic foam*. Smart Structures and Materials **13**, 49 (2004).
- [3] W. R. Powers. US Patent 3 025 200 (1962).

ATOMIC-SCALE MODELLING OF PLASTIC DEFORMATION OF NANOCRYSTALLINE COPPER

J. Schiøtz

Center for Atomic-scale Materials Physics, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby

Using large-scale molecular dynamics, we have performed atomic-scale simulations of nanocrystalline copper with grain sizes from 5 to 50 nm. The simulations show a clear maximum in the flow stress when the grains are 10-15 nm in diameter. At this grain size, there is a shift in deformation mechanism, from dislocation-mediated plasticity at larger grain sizes to grain boundary sliding at smaller. Above the maximum in hardness, the grain size dependence of the hardness is consistent with the Hall-Petch relation, stating that the hardness scales inversely with the square root of the grain size. Below the maximum in hardness, the large density of grain boundaries prevents dislocations from contributing significantly to plasticity, but instead the grain boundaries themselves carry the deformation.

The Hall-Petch relation is normally explained by the creation of dislocation pileups in the grains. It has not been clear if this explanation of the Hall-Petch effect is valid for sub-micrometer grains, but the simulations presented here clearly show the existence of pileups in the simulation with average grain size of 50 nm. The dislocation dynamics in the grains is dominated by the grain boundaries, as almost all dislocation nucleation occurs at the grain boundaries, which also act as efficient dislocation sinks. During the plastic deformation, a large number of stacking faults and a much lower number of twin boundaries are created. These do not contribute significantly to the flow stress, as no work hardening is seen whereas the number of stacking faults increases with strain.

THIN AL-LAYERS SPUTTERED ONTO POLYIMID - AN AUXETICS?

J. Schreiber and V. Melov

*Fraunhofer Institute for Nondestructive Testing, Branch Lab EADQ Dresden
Krügerstrasse 22, D-01326 Dresden, Germany*

The downscaling of device size, which is characteristic for recent developments in micro-systems engineering, causes a significant modification of the material properties. For instance, a qualitatively new mechanical behavior was identified for micro-structured metallic systems like Al- and Cu-lines [1]. This behavior can be characterized by a 1D-elastic and 2D-plastic response until reaching a strain limit at which the conventional 3D-elastic-plastic behavior sets in. This anomalous behavior was found only for coarse grained lines with grain sizes in the order of line width respectively thickness. The consequences of such behavior for mechanical stability e.g. of micro-mirrors, which are employed in spatial light modulators of mask-less scanners for wafer patterning, are currently investigated (see [2]).

In this context, tensile testing experiments and measurements of the intrinsic stresses as a function of the strain were performed to determine the macroscopic elastic constants for Al-layers deposited onto different substrates. For that purpose the macro-stress in the Al-layer was calculated in the framework of a planar model [3] for a fixed radius of a stripe like sample, which was bended with a four point bending machine. In the case of a 50 nm thick Al-layer on a Si-wafer, fiber texture was found, a Youngs module of $E = 80$ GPa and the Poisson ratio $\nu = 0.35$ were obtained. Otherwise strange behavior was recognized for a 200 nm Al-layer sputtered onto Polyimid resist of 670 nm thickness on a Si-wafer. A good fit for the X-ray data could be reached by $E = 9$ GPa and $\nu = -0.95$.

A possible explanation of such behavior is the existence of self organized vortex-like structures of Al grains of about 20 nm size. The macroscopic elastic response of those correlated elements of a meso-structure could be described mainly by soft elastic grain boundary movements, but with an expansion of the vortex in several directions in correspondence with a negative Poisson number. Further load experiments and microscopic investigations are planned to prove the proposed structural model and to verify the membership of Al-layers sputtered onto Polyimid substrate to the world of auxetics.

References

- [1] B. Bendjus, B. Köhler, V. Melov, and J. Schreiber, *Materials Science and Testing Issues in Developing Microstructured Metallic Systems*, Proceedings of Materials Week, 2002, p.387.
- [2] J. Schreiber, St. Braun, A. Gatto, and H. Schenk, *Testing, Reliability, and Application of Micro- and Nanomaterial Systems*, Paper presented at SPIE conference in San Diego, March 2004, to be published.
- [3] T. Iancu *Calculation of thermal residual stress fields in ceramic-metal compounds*, Fortschrittsberichte VDI, Reihe 18: Mechanik/Bruchmechanik, Nr. 74 (VDI-Verlag, Düsseldorf, 1989).

AUXETIC BEHAVIOUR: APPEARANCE AND ENGINEERING APPLICATIONS

G. E. Stavroulakis

University of Ioannina, Greece and Technical University of Braunschweig, Germany

Materials with negative Poisson's ratio are known as auxetic. This behaviour can be attributed to micromechanical properties like nonconvex microstructures, therefore may be studied within some limits with methods of structural analysis.

The presentation will start with a review of auxetic behaviour and a short discussion of their possible applications. Then, numerical schemes suitable for the numerical prediction of auxetic behaviour and its study, based on numerical homogenization techniques will be presented (see [1-2] for relevant results in statics). Optimal design of microstructures, so that the resulting material has a wished auxetic behaviour, and optimal design of structures with variable material behaviour (including auxetic) will be discussed in the next part of the presentation. First results in this direction have been published in [3-4], while a more general theoretical framework based on nonconvex optimization techniques can be found in [5]. Finally, possible extensions to dynamics and open problems will be briefly addressed.

References:

- [1] P. S. Theocaris, G. E. Stavroulakis, P. D. Panagiotopoulos, *Negative Poisson's ratio in materials with a star-shaped microstructure. A numerical homogenization approach*, Archive of Applied Mechanics (Ingenieur Archiv) **67(4)**, 274 (1997).
- [2] P. S. Theocaris, G. E. Stavroulakis, *The homogenization method for the study of variation of Poisson's ratio in fiber composites*, Archive of Applied Mechanics (Ingenieur Archiv) **68(3/4)**, 281 (1998).
- [3] P. S. Theocaris, G. E. Stavroulakis, *Multilevel, iterative optimal design of composite structures, including materials with negative Poisson's ratio*, Structural Optimization **15(1)**, 8 (1998).
- [4] P. S. Theocaris, G. E. Stavroulakis, *Optimal Material Design in Composites: An Iterative Approach Based on Homogenized Cells*, Computer Methods in Applied Mechanics and Engineering **169(1-2)**, 31 (1999).
- [5] E. S. Mistakidis, G. E. Stavroulakis, *Nonconvex optimization in mechanics. Algorithms, heuristics and engineering applications by F.E.M.*, Kluwer Academic Publishers, Dordrecht, Boston, London 1998.

AL-BASED SYSTEMS WITH UNUSUAL MECHANICAL AND TRANSPORT PROPERTIES

K. Müllerová^{1,3}, F. Simančík^{1,3}, P. Švec^{2,3}

¹ *Institute of Materials and Machine Mechanics, Slovak Academy of Sciences, Bratislava*

² *Institute of Physics, Slovak Academy of Sciences, Bratislava*

³ *“NanoSmart”, Center of Excellence of the Slovak Academy of Sciences*

Addition of selected transition-metal elements into aluminum matrix is known to yield systems which exhibit unique mechanical properties, especially high yield strength obtained after suitable heat treatment. These lightweight systems are known to be compactable from ribbon shape prepared by rapid quenching of the melt into bulk form, yielding physically and technically attractive materials.

The investigation of physical causes for enhancement of mechanical properties will be focused on formation of special short-range ordering leading to the desired effect and to the potential for compaction by methods preserving such structure. The influence of heat treatment of both the melt and rapidly quenched ribbons will be correlated with local ordering and presence of structures with unit cells containing high number of atoms and having nonperiodic/quasicrystalline structure. Special structures formed will be analyzed by the methods of kinetic and structural analysis using electron microscopy and X-ray diffraction along with the evolution of electrical resistivity in time and temperature. The results will be correlated with the presence and persistence of the nanograined Al phase containing both intermetallic and quasicrystalline phases with increased structural stability.

Formation of bulks by specialized techniques will be presented, emphasizing on one side high-density systems prepared by hot-pressing or sintering and on the other side highly porous foam systems with closed pore structure. Internal structure and crystalline phase formation will be correlated with qualitative differences in mechanical properties due to the effects of pore structure, pore content and average sample density.

STEREOGRAPHIC PROJECTIONS OF POISSON'S RATIO IN AUXETIC CRYSTALS

S. P. Tokmakova

N. N. Andreev Acoustics Institute, 117036, Russia, Moscow, Shvernika 4

Anisotropy is the reason for the negative Poisson's ratio in crystals. Crystals with negative Poisson's ratio may be considered as a 3-D natural anisotropic dense structure with auxetic behavior. The auxetic behavior in some cubic metals for a stretch along a cube-face diagonal was investigated in details by R.H.Baughman et al., F.Milstein, K.Huang, M.Jain, M.P.Verma. These authors considered directions with the extremes values of Poisson's ratio in crystal for a stretch along a cube-face diagonal and lateral strain along the orthogonal cube-face diagonal and along the cube-axis. In this paper the stereographic projections of Poisson's ratio for a set of crystals with cubic, hexagonal and monoclinic symmetry were computed. From these stereographic projections the Poisson's ratio for any possible directions of stretch and lateral strain in crystal were calculated and orientations of stretch and lateral strain with extremes values of Poisson's ratio were obtained. Crystals with auxetic behavior (with negative values of Poisson's ratio) were revealed. Orientations of stretch directions and lateral strain directions with negative values of Poisson's ratio were determined. By analysis of the above results cuts with optimal negative values of Poisson's ratio were revealed in zinc, molybdenum sulfide, carbon, graphite, polypropylene, monoclinic natural minerals labradorite and augite, complex silicate and in a set of cubic alloys. Peculiarities of the acoustic properties of cubic crystals with negative Poisson's ratio were studied. The exotic behavior of change of cross-section of cylindrical rod during the stretching along the rod axis was revealed in naturally occurring mineral cristobalite SiO₂ – an example of molecular auxetics. The elastic modules of crystals from the manual of Landolt-Bornstein were used in calculations.

References

- [1] F. Milstein and K. Huang, *Existence of a negative Poisson's ratio in fcc crystals*, Phys. Rev. B **19**, 2030 (1979).
- [2] J. Manjula and M. P. Verma, *Poisson's ratios in cubic crystals corresponding to (110) loading*, Indian Journal of Pure and Applied Physics **28**, 178 (1990).
- [3] R. H. Baughman, J. M. Shacklette, S. Stafstrom, A. A. Zakhidov, T. B. Mitchell, and D. H. E. Dubin, *Negative Poisson's ratio as a common feature of cubic crystals*, Science **288**, 2018 (2000).
- [4] S. P. Tokmakova, *Cuts with negative Poisson's ratio in crystals in Nonlinear Acoustics at the beginning of the 21-th Century*, Proceedings of the 16-th International Symposium on Nonlinear Acoustics, Eds. O. V. Rudenko, and O. A. Sapozhnikov, (Faculty of Physics, MGU, Moscow, 2002) vol.2, pp. 669-672.
- [5] Landolt – Bornstein, *Numerical Data and Functional Relationships in Science and Technology*, 1984, New Series, Group III, V.18, V.29(A) Springer, Berlin/New York.

MONTE CARLO SIMULATIONS OF HARD BODY SYSTEMS WITH EXTREME VALUES OF THE POISSON RATIO

K. V. Tretiakov^{1,2} and K. W. Wojciechowski¹

¹ *Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, 60-179 Poznan, Poland*

² *The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11 I-34014 Trieste, Italy*

Hard body systems are the simplest systems which can model short-range molecular correlations. Interacting by the hard body potentials, infinite when any two bodies overlap and zero otherwise, these systems mimic steric hindrances which influence the motion of any molecule and which are caused by molecular cores of neighbouring molecules. Moreover, being athermal, the hard body systems allow one for direct studies of entropic effects which in usual 'energetic' models are concealed under cover of energy. For this reason these systems play an important role in modeling condensed matter phases like liquids, liquid crystals, plastic crystals and solids. They can be also used for modeling granular systems.

It is well known that molecular shape plays a significant role in defining thermodynamic and structural properties of a many body system. In particular, one can show that elastic properties of the system are strongly influenced by the molecular shape and for certain molecular shapes the system can exhibit negative Poisson ratio. It is then interesting to study elastic properties of various hard body systems [1].

In this lecture we review extensive numerical studies of elastic properties of some model systems which reveal extreme values of the Poisson ratio. The simulations were performed by the Monte Carlo method in the NpT ensemble with variable shape of the periodic box. We consider the homomolecular systems of cyclic pentamers, hexamers and heptamers. We present also the polydisperse hard disc systems in two dimensions and the polydisperse hard sphere system in three dimensions.

For all the systems studied we observed that the Poisson ratio shows some extreme values. For the cyclic multimers (pentamer, hexamer, heptamer) the extreme (positive or negative) values of the Poisson ratio are obtained at the phase transitions. It is worth to add here that the Poisson ratio has occurred to be very sensitive indicator of both the structural (e.g. orientational order) changes and the interaction mode changes.

In systems of hard discs and hard spheres presence of the size polydispersity leads to growth of the Poisson ratio with increasing density. Thus, the Poisson ratio of polydisperse systems of spherically symmetric hard particles reaches its extreme value at the close packing limit. The observed extremum is a maximum what is in contrast to the monodisperse systems of hard spheres and hard discs for which the Poisson ratio reaches its minimum value.

For all the hard body systems studied the elastic properties in the vicinity of the close packing can be described by a very simple approximation known as the free volume theory.

References

- [1] K. W. Wojciechowski, K. V. Tretyakov, and M. Kowalik, *Phys. Rev. E* **67**, 036121 (2003).

MODELLING OF ONE, TWO AND THREE DIMENSIONAL MOLECULAR AUXETICS

G. Y. Wei

Department of Polymer Science and Engineering, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, P R CHINA

We report recent progress in computer modeling of molecular auxetics with particular attention paid to the so-called auxegen-approach developed in our laboratory. Several design routes of this new approach are presented with specific examples. The approach may provide a new route to synthesize high-strength auxetic polymers [1,2].

The *auxegen* as coined by Wei and Feng [3] in 1998 has the meaning of anything or more specifically any molecule that generates auxeticity in any d -dimensional network or lattice formed from it. It has its origin in the repeating structure unit of the auxetic honeycomb molecule though it differs from the latter in that it is itself a molecule that interacts with its neighbors only through van der Waals forces or H-bonds. For the latter case, the auxegen is equivalent to the repeating cell unit of a regular supramolecular network or supermolecule, and such a 1D auxetic supermolecule is just a non-covalently-bonded polymer. Obviously, the word *dimensionality* or the symbol d used here refers only to the number of mutually orthogonal spatial directions in which any molecular auxetics shows auxeticity when stretched or periodicity in terms of the network structure.

If such auxegens are randomly or regularly dispersed by chemical means in a solid medium such as an elastomer, a nano- or molecular composite results, which may be either auxetic or non-auxetic depending on factors like volume fractions and modulus ratios of the component phases [4,5]. We note that the above definition of auxegen does not allow Wojciechowski's interpenetrable hexmer [6] to be called auxegen though it may be regarded as the first example of "imaginary auxegens." Furthermore properly-end-capped re-entrant honeycomb cell unit (RHCU) [7,8] and Rothenburg *et al*'s dilational equilateral triangular cell unit [9] are among the earliest examples of real auxegens that may be experimentally synthesized.

In principle, there exist an unlimited number of auxegens with all possible molecular configurations. But we found that those based on RHCU are the most convenient to start with at least computationally if not experimentally. We have designed a variety of such auxegens having linkages like $-C\Box C-$, $-Ph-$, $-COO-$, $-CONH-$ and $-O-$, and also carried out the modeling work on their 3D elasticity calculations [10-13]. The results show that most of them exhibit auxeticity in at least one plane, say xoy plane which takes up a larger part of the projection of the planar auxegen, with one special case of a 2D supramolecule formed by connecting sidewise specially-designed copolymers through H-bonds showing a negative Poisson ratio as negatively large as -11 .

References

- [1] R Lakes, *Science* **235**, 1038 (1987) ; *ibid*, 1987 **238**, 551 (1987), US 4668557, 1987
- [2] K. E. Evans and A. Alderson, *Adv. Mater.* **12**, 617 (2000).
- [3] G. Y. Wei and X. D. Feng, P&G (Cincinnati, USA), unpublished results, (1998).
- [4] G. Y. Wei and S. F. Edwards, *Comput Polym Sci.* **2**, 44 (1992).
- [5] G. Y. Wei and S. F. Edwards, *Phys. Rev. E* **58**, 6173 (1998); *Physica A* **258**, 5 (1998).
- [6] K. W. Wojciechowski, *Phys Lett A* **137**, 60 (1989).
- [7] G. Y. Wei, S. F. Edwards, I. J. Hutchinson, W. C. Mackrodt, S. C. Rogers, K. E. Evens, ICI Chemicals and Polymers (Runcorn, UK), unpublished results, (1991).
- [8] K. E. Evans, M. A. Nkansah, I. J. Hutchinson, and S. C. Rogers, *Nature* **353**, 124 (1991).
- [9] L. Rothenburg, Berlin AI AI, R. J. Bathurst, *Nature*, **354**, 470 (1991).
- [10] G. Y. Wei, H. M. Wu, X. R. Xu, J. Y. Yuan, W. X. Cao, and X. D. Feng, P&G Asia (Tokyo, Japan), unpublished results, (2001).
- [11] G. Y. Wei, *Mater Rev. (Beijing)*, **17**, 8 (2003).
- [12] H. M. Wu, *Molecular Design of Auxetic Networks, Auxogens, and Auxetic Polymers and Supermolecules*. PhD Dissertation, Peking University, (2003).
- [13] H. M. Wu and G. Y. Wei, *Acta Polym Sin.*, **2**, 201 (2004); *Chin. J. Polym. Sci.*, (2004), in press (to appear in the June issue).

SIMPLE MECHANISMS LEADING TO $\nu < 0$

K. W. Wojciechowski

*Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17,
60-179 Poznań, Poland*

Materials showing negative Poisson ratio, known also as auxetics, increase (decrease) their transverse dimensions when pulled (pushed) longitudinally. The simplest mechanisms leading to this very counterintuitive behaviour have been suggested by Almgren and by Kolpakov already in 1985. The Almgren's idea consists in exploiting a collective rotation of a system of rigid bodies connected by vertices. The solution proposed by Kolpakov is based on fixing mutual orientations of objects which, however, can easily change their (linear) size. In both the cases it is possible to change the size of a sample without changing its shape, i.e. to obtain the Poisson ratio -1 . Various artificial structures, which base on these mechanisms, or their 'mixtures', as well as on some other mechanisms, have been designed and manufactured since that time; the first was produced by Lakes in 1987. Such structures can be built on various length scales, from the macro- to the micro-scale.

For many applications it is preferable to have a uniform structure down to the micro-level. Thus, it is natural that some efforts have been undertaken to obtain microscopic structures showing negative Poisson ratio. Most of them were based on building some artificial structures, which are typically not stable from the point of view of the thermodynamics. (Such systems will be further referred to as structural or artificial auxetics.) However, instead of using the above mentioned approach, one can try to search for molecules which will form thermodynamically stable auxetic phases. (Such systems will be further referred to as molecular auxetics.) Searching for such molecules is one of the subjects of the present lecture. In particular, a simple molecular model system will be presented which reveals an interesting relation existing between the mechanisms proposed by Almgren and Kolpakov.

Understanding of the thermodynamic stability of various systems requires not only analysis of their energetic properties but also some knowledge on their entropic properties. Thus, hard body systems, which are 'governed' by the entropy alone, are of interest and importance in this aspect. Some examples will be given.

Various systems can become auxetic in certain regions of the parameters (e.g. thermodynamic ones) describing them. It can be shown that negative pressure is one of such parameters. It will be briefly explained why it is so. Changing parameters describing a system allows for *switching* from a common to an auxetic behaviour. (This can find practical applications.) An example of such a system, for which the temperature plays the role of the switching parameter, will be shown.

Some other mechanisms, which can be used to obtain an auxetic behaviour, will be mentioned and discussed briefly. They have been found by applying a simple scheme for a systematic search for auxetic systems; the scheme is based on analysis of the conditions sufficient for obtaining the Cauchy relations for the elastic constants of systems under study.

POSTERS

SIMULATION OF THERMAL PROPERTIES OF MATERIALS USING ATOMISTIC AND CONTINUUM MODELS

W. Alda¹, M. Białoskórski², R. Górecki¹ and J. Rybicki²

¹ *AGH University of Science and Technology, Mickiewicza 30, 30-059 Kraków*

² *Gdansk University of Technology, Faculty of Technical Physics and Applied Mathematics, Narutowicza 11/12, 80-952 Gdańsk and TASK Computer Centre, Narutowicza 11/12, 80-952 Gdańsk*

In the poster we present the model and the simulation results of heat transfer in 2D plates modeled both by atomistic and continuum systems. First we analyze the heat transfer in the models treated separately. In the particle model we use non-equilibrium molecular dynamics with two heat baths placed on the ends of the system. According to the results from discrete system we adjust specific parameters of the continuous FEM model in order to obtain comparable results. In the next step we couple atomistic and continuum models through a bridging domain with an overlapping region in which Hamiltonian is a combination Hamiltonians in both models. Special attention has been paid to the analysis of the influence of the grid scale and the integration time-step in the continuum system, in order to enable smooth energy transfer and avoid rapid growth of energy in the atomistic part near the particle-continuum boundary.

The work has been supported by KBN, grant 7 T11F 013 21. The calculations have been performed at the TASK Computer Centre (Gdansk, Poland) and at CYFRONET (Kraków, Poland).

DISTRIBUTIONS OF DISTORTION PARAMETERS VALUES FOR SEVERAL PROTOTYPICAL STRUCTURAL UNITS IN COMPUTER-SIMULATED MATERIALS

G. Bergmański¹ and J. Rybicki^{1,2}

¹ *Department of Solid State Physics, Faculty of Technical Physics and Applied Mathematics, Gdansk University of Technology, Narutowicza 11/12, 80-952 Gdansk, Poland*

² *TASK Computer Centre, Narutowicza 11//12, 80-952 Gdansk, Poland*

We have calculated and discussed distributions of values of several shape estimators in the function of the distortion degree for a series of typical structural units in computer simulated solids. The paper's aim is to provide reference data useful in quantitative analysis of the short-range structure in computer-simulated materials. We illustrate our approach with an example related to the structure of borate glasses. Although the B_2O_3 glass has been known for many years and has found many important practical applications (e.g. in optical fibre technology), its structure is still intensively investigated and several open questions concerning the structure of B_2O_3 still remain. We use one of our shape estimators for BO_3 triangles in borate glasses, simulated with various force fields. We compare the results both with experimental data and theoretical predictions and critically appraise reliability of the applied interatomic interactions.

The work has been supported by KBN, grant 7 T11F 013 21. The calculations have been performed at the TASK Computer Centre, Gdansk, Poland.

AN INTEGRATED QUANTUM-CLASSICAL SIMULATION METHOD FOR OPTIMIZATION OF CRYSTAL LATTICE OF HEAVY METAL SOLIDS

M. Bobrowski^{1,2}, J. Dziejczak¹, D. Kubacki¹, and J. Rybicki^{1,2}

¹ *Department of Solid State Physics, Faculty of Technical Physics and Applied Mathematics, Gdansk University of Technology, Narutowicza 11/12, 80-952 Gdansk, Poland*

² *Academic Computer Center TASK, Narutowicza 11/12, 80-952 Gdansk, Poland.*

A computational scheme integrating quantum mechanical (QM) and classical molecular dynamics (MD) methods is presented. The system is divided into two regions treated at different level of theory: electronic states are taken into account in one part and atomic motions in the second.

In addition, a method for interfacing the two regions is applied; an interface between the QM and MD region consists of parametrized atoms included into the QM part. When a simple method based on hydrogen link atoms is applied, it fails when we try to optimize deformed lattice of electronically delocalized systems, such as graphite or heavy metals.

We use not only hydrogen-like atoms in the interface but also atoms with higher angular momentum orbitals as well as specific parameters in semiempirical tight-binding (TB) algorithms in QM region to describe well properties of such electronically delocalized systems.

The work has been supported by grant 1663/T11/2001/21 from the Polish State Committee for Scientific Research. Calculations were carried out with the use of the resources and software at the TASK Computer Centre.

ANOMALOUS SOFTNESS "COMPRESSIBILITY" OF INVERSE POWER SYSTEMS

A. C. Brańka¹ and D. M. Heyes²

¹ *Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, 60-179
Poznań, Poland*

² *Chemistry Division, School of Biomedical and Molecular Sciences, University of
Surrey, Guildford GU2 7XH, UK.*

We recently proposed a simple analytic equation of state for a generic fluid composed of particles interacting via the inverse power, r^{-n} potential [A.C. Brańka and D.M. Heyes, Mol. Phys. 2004, in press]. Our equation of state is accurate for n -values greater than about 18, when compared with our Molecular Dynamics simulation data. It is informative to consider the compressibility factor, Z , as a function of density, ζ , and softness, $1/n$. In this previous study we showed that in the $\zeta; 1/n$ plane, $Z(\zeta; 1/n)$ has two well defined regions, characterized by either a positive or negative value of the function, $\chi = 1/(\partial Z/\partial \varepsilon)_\zeta$, where $\varepsilon = 1/n$. χ is a kind of 'compressibility', where $1/n$ takes the place of volume.

We have performed some new simulations, this time extending them into the (fcc) solid part of the phase diagram. These simulations show that this χ variation extends into the solid phase. For $n \geq 20$ there exists a region in the $(\zeta; \varepsilon)$ plane where $(\partial Z/\partial \varepsilon)_\zeta < 0$.

In the presentation these trends in χ and the accompanying demarcation or maximum pressure line are discussed.

RELAXATION KINETICS OF AMORPHOUS Fe₄₁Ni₄₀Zr₇B₁₂ ALLOY

S. Kostyrya, Z. Śniadecki and B. Idzikowski

Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, 60-179 Poznań, Poland

The devitrification of melt-spun amorphous ribbons is usually a multistage process. The structural transformations of Fe₄₁Ni₄₀Zr₇B₁₂ ribbon during heat treatment show formation of the nanosized α -Fe and/or fcc-(Fe, Ni)₂₃B₆ grains placed in amorphous matrix [1]. Those alloys shows an interesting relaxation effect after annealing at temperature below crystallization onset which is usually connected with considerable decrease of Curie temperature. After such annealing those ribbons are still fully amorphous. An amorphous melt-spun ribbons exhibits in as-quenched state local heterogeneities in density [2] removable by long-term annealing at relative low temperatures. The determination of mechanical strains in the alloys can be made by investigation of structural relaxation processes.

This paper describes relaxation kinetics of Fe₄₁Ni₄₀Zr₇B₁₂ amorphous alloys. The thermokinetical parameters of the structural relaxation was determined experimentally from differential scanning calorimetry (DSC) measurements under linear-heating (in the wide range heating rates 10-50 K/s) in protective argon atmosphere. Activation energy of relaxation and diffusion coefficient under continuous heating at constant rate was estimated by Kissinger's method [3]. XRD measurements using Co $K\alpha$ radiation were applied for identification of amorphous structure as well as crystallization products.

The magnetic behavior of such materials was described earlier and compared with theoretical calculations [4]. After annealing, ribbons became magnetically soft and in a nanocrystalline state show also good mechanical properties, as compared with the FINEMET, NANOPERM or HITPERM.

References

- [1] B. Idzikowski, J.-M. Greneche, A. Szajek, and J. Kovač, *Appl. Phys. Lett.* (2004), in print
- [2] T. Egami, *Atomic short-range ordering in amorphous metal alloys*, in F.E. Luborski (ed.) *Amorphous Metallic Alloys*, Butterworths monographs in materials, 1983
- [3] H. G. Kissinger, *J. Res. Natl. Bur. Stand.* **57**, 217 (1956)
- [4] B. Idzikowski and A. Szajek, *Mater. Sci.* **21**, 73 (2003)

MONTE CARLO SIMULATIONS OF ELASTIC PROPERTIES OF APERIODIC CRYSTALS OF RIGID DIMERS AND TRIMERS IN THREE DIMENSIONS

M. Kowalik and K. W. Wojciechowski

Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, 60-179 Poznań, Poland

Recently, systematic studies of various mechanisms which may lead to negative Poisson ratio have been proposed [1]. One of possibilities to obtain negative Poisson ratio is by using assemblies of nonconvex objects [2-8]. Examples of nonconvex objects can be obtained by 'sticking' together hard discs (in two dimensions) or hard spheres (in three dimensions). In the simplest cases one obtains hard dimers and hard cyclic trimers, respectively consisting of two and three hard discs/spheres, further referred to as 'atoms'. Encouraged by the results obtained in two dimensions [9,10] we performed extensive computer simulations of their three-dimensional counterparts which are the subject of the present contribution.

As it occurs in two dimensions, also in three dimensions both the hard dimer and the hard trimer molecules can form structures corresponding to the close packing of the atoms. Thus, the spheres-atoms form the fcc regular lattice at close packing [11], whereas the molecular arrangements are not periodic. The *aperiodic* molecular ordering characterizes also the thermodynamically stable solid phases in both the studied cases [12,13] and implies the effective cubic symmetry of these systems. Their elastic properties are fully described by only three elastic constants.

Results concerning the equation of state and the elastic properties of the hard dimers and trimers, studied by a version [14] of the constant pressure Monte Carlo method with variable shape of the box, are presented. Influence of defects (vacancies) on the Poisson ratio in these systems is also discussed.

References

- [1] K. W. Wojciechowski, in *Properties and Applications of Nanocrystalline Alloys from Amorphous Precursors*, edited by B. Idzikowski, P. Svec, M. Miglierini (Kluwer Academic Publishers, Dordrecht, 2004), in print.
- [2] R. F. Almgren, *Journal of Elasticity* **15**, 427 (1985).
- [3] A. G. Kolpakov, *Prikl. Matem. Mekhan.* **49**, 969 (1985).
- [4] R. Lakes, *Science* **235**, 1038 (1987).
- [5] K. W. Wojciechowski, *Molec. Phys.* **61**, 1247 (1987).
- [6] G. Wei, *J. Chem. Phys.* **96**, 3226 (1992).
- [7] G. W. Milton, *J. Mech. Phys. Solids* **40**, 1105 (1992).
- [8] P. S. Theocaris, G. E. Stavroulakis, P. D. Panagiotopoulos, *Archive of Applied Mechanics* **67**, 274 (1997).
- [9] K. V. Tretiakov and K. W. Wojciechowski, *Elastic properties of the aperiodic solid phase of two-dimensional hard dimers*, to be published.
- [10] K. W. Wojciechowski and K. V. Tretiakov, *Negative Poisson ratio of the aperiodic solid of two-dimensional trimers*, to be published.

- [11] T. C. Hales and S. P. Ferguson, <http://www.math.lsa.umich.edu/~hales/countdown/>.
- [12] C. Vega, E. P. A. Paras, and P. A. Monson, *J. Chem. Phys.* **96**, 9060 (1992).
- [13] M. Kowalik and K. W. Wojciechowski, *Equation of state of the hard cyclic trimers in three dimensions*, in preparation.
- [14] K. W. Wojciechowski, *Computational Methods in Science and Technology* **8(2)**, 77 (2002).

RADIAL DISTRIBUTION FUNCTION (RDF) AND STATE EQUATION FOR BINARY HARD SPHERE MIXTURES OBTAINED FROM COMPUTER SIMULATION (MD)

B. Kuroczycki, M. Banaszak, S. Jurga

³ *Department of Macromolecular Physics, Adam Mickiewicz University, Poznan, Poland*

Computer simulation is a very important tool in research of colloidal suspensions, melts and other mixtures. In this work, we use Molecular Dynamics (MD) simulation for binary hard sphere mixtures, i.e., a system consisting of many small spheres surrounding a few large spheres.

Hydrodynamic interactions between large spheres (mediated by small spheres) originate from the above model system. We don't use any approximation such as Onseen's Tensor etc.. Static and dynamics properties of colloidal suspension are similar to those of the behaviour of simple fluid. Especially phase transitions in the simple fluid can be compared to the phase transitions in our binary mixtures (fluid -> glass -> crystal). However, diffusivity relaxation times for fluid molecules are about 10^9 larger than relaxation times of molecules in suspensions. In this way, lifetime of the metastable phase of suspension observed before crystallization, can be long enough (from minute to hours) to allow experimental studies. This long time gives possibility to accurately measure physical properties in this state [2]. Colloidal suspension can be studied by many experimental methods such as: Rheological experiments (viscosity and elastic properties), light scattering (structural properties and diffusion coefficients) and NMR (memory coefficients and structure relaxation).

Representative materials used in the experiment, comprised of cores of polymethylmetacrylate (PMMA) stabilized by thin layers of poly-12-hydroxystearic acid and suspended in cis-decalin [3]. In this simulation we record the radial distribution function (RDF) and the equation of state (EoS) data. The results are compared to Monte Carlo (MC) simulations [1] and theoretical results (BMSCL, HC, SYH,ML) [1].

References

- [1] P. N. Pusey and W. Van Megen, *Observation of Glass Transition in Suspension of Spherical Colloidal Particles*, Phys. Rev. Lett. **59(18)**, 2083 (1987)
- [2] P. N. Segre, S. P. Meeker, P. N. Pusey, and W. C. Poon, *Viscosity and Structural Relaxation in Suspensions of Hard-Sphere Colloids*, Phys. Rev. Lett. **57(5)**, 958 (1995).
- [3] D. Cao, K. Y. Chan, D. Henderson, W. Wang, *Monte Carlo data of dilute solutions of large spheres in binary hard sphere mixtures*, Molec. Phys. **98(9)**, 619 (2000).
- [4] M. P. Allen, D. J. Tildesley, *Computer Simulation of Liquids*, Calderon Press, Oxford (1996)

ON THE NEGATIVE POISSON RATIO OF COMPOSITES OF FRACTAL STRUCTURES

V. V. Novikov¹, K. W. Wojciechowski² and A. V. Novikov¹

¹ *Odessa National Polytechnical University, 1 Shevchenko Prospekt, 65044 Odessa, Ukraine*

² *Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, 60-179 Poznań, Poland*

Hierarchic model of structure [1] is applied to study the Poisson ratio of a two-component inhomogeneous medium with chaotic, fractal structure. Elastic properties of non-uniform, two-component systems are studied in frames of a model of percolation on a simple cubic lattice. It is shown that as the ratio of the bulk moduli of the components tends to zero, $k_2/k_1 \rightarrow 0$ (where 1,2 denote the harder and softer phase, respectively), the Poisson ratio of the system tends to 0.2 at the percolation threshold of the harder phase, no matter what the values are of the Poisson ratios of the components. The Poisson ratio calculated for the hierarchic model is compared with the Poisson ratio calculated for the well known Hashin-Shtrikman model.

A qualitatively new, collective mechanism leading to negative Poisson ratio is suggested [2,3] which bases on a relation between the ratio of the elastic constants at the percolation threshold and the lattice coordination number.

References

- [1] V. V. Novikov, K. W. Wojciechowski, D. V. Belov, and V. P. Privalko, *Phys. Rev. E* **63**, 036120 (2001).
- [2] V. V. Novikov and K. W. Wojciechowski, *Physics of the Solid State* **41**, 1970 (1999).
- [3] K. W. Wojciechowski and V. V. Novikov, *Task Quarterly* **5**, 5 (2001).

NUMERICAL AND EXPERIMENTAL STUDY OF AUXETIC CLOSED-CELL FOAMS

S. V. Shilko, D. A. Konyok

Metal-Polymer Research Institute, National Academy of Sciences, Gomel, Belarussia

The procedures of fabrication and testing of auxetic foams with closed cells based on foaming a liquid substance or by microspheres joining are discussed. Physically, to obtain auxetic structure, the bending rigidity of elastic rods, plates and shells should strongly depend on the initial curvature. The cells of small size are found mostly to hold their original shape. Large ones show relatively low rigidity, and would get deformed similarly to thin-walled shells when compressed with a possibility of losing stability. Thus, the volumetric compression of a foamed material is mainly realized at the expense of decreased free volume of large cells. Separation of cells according to deformation levels is found to cause auxetic elastic behavior in converted closed cells foams.

Technologically, to obtain this auxetics we proposed a two-stage process. It includes the formation of concave cell structure by permanent volumetric compression of initial material just after foaming in the solidification state under action of a liquid or gas. High plasticity of foam materials in this stage allows us to obtain the re-entrant structure of cells. We produce the effective method to obtain material with non-convex cells mostly using the gas or liquid under pressure as forming instrument. After cooling the foam material shows the property of elastic (reversible) deformation. The homogeneity and isotropy of Poisson's ratio of obtained auxetics are caused by uniform distribution of the gas or liquid pressure on the sample surface.

Some difficulties of experimental determination of Poisson's ratio are caused by complex geometry of sample boundaries. One may avoid this obstacle by means of computer analysis. The procedure we used includes the obtaining the images of material's structure with the help of digital videocamera before and after deformation. And then we use numerical analysis of difference of these images for the Poisson's ratio calculation. Some problems of the Poisson's ratio minimization for foam materials we have solved by using finite element analysis.

ON THE CONTRIBUTION OF AN ELASTIC COMPONENT TO CRYSTAL GROWTH IN COMPLEX ENVIRONMENTS

J. Siódmiak and A. Gadomski

*Institute of Mathematics and Physics, University of Technology and Agriculture,
Kaliskiego 7, 85-796 Bydgoszcz, Poland*

Based on simple statistical-mechanical models, we consider how elastic interactions between a crystal and its surroundings change crystal growing conditions. First, we analyze the influence of some modification of the Gibbs-Thomson thermodynamic condition, prescribed at the crystal boundary [1,2], on some properties of a kinetic model of protein crystal growth in mass convection regime [3], where a crystal grows on a single nucleus. Second, we argue whether certain growing conditions of percolation type, typically characteristic of some polycrystals or bubbles [4] may contain a possibility of anomalous viscoelastic behavior [5-7]. (Here a many-nuclei system is taken into consideration.) Whenever possible, we make use of late-time growing conditions; we also refer to typically slow growing conditions in the systems under consideration.

Applications of the proposed modeling, preferentially to inhomogeneous and two- or many-component soft or jammed materials, are discussed.

References

- [1] J. Schmelzer and I. Gutzow, Rostock. Phys. Manusk. **13**, 82 (1989).
- [2] J. Schmelzer, J. Möller, V. V. Slezov, I. Gutzow, and R. Pascova, Quimica Nova **21**, 529 (1998).
- [3] A. Gadomski and J. Siódmiak, Cryst. Res. Technol. **37**, 281 (2002).
- [4] A. Gadomski, Physica A **274**, 325 (1999)
- [5] V. V. Novikov, K. W. Wojciechowski, D. V. Belov, V. P. Privalko, Phys. Rev. E, **63**, 036120 (2001)
- [6] V. V. Novikov and K. W. Wojciechowski, Physics of the Solid State **41**, 1970 (1999).
- [7] K. W. Wojciechowski, V. V. Novikov, Task Quarterly **5**, 5 (2001).

LOW-TEMPERATURE ORDERING EFFECTS IN SYMMETRIC DIBLOCK COPOLYMER MELTS FROM LATTICE MONTE CARLO SIMULATION

S. Wołoszczuk, M. Banaszak, S. Jurga and T. Pakula

*Department of Macromolecular Physics, Adam Mickiewicz University, Umultowska 85,
61-614 Poznań, Poland*

Monte Carlo simulations, using the Cooperative Motion Algorithm, have been performed to investigate the behaviour of symmetric diblock melts [3] and the corresponding A-B-A triblock [1,2] copolymer melts. In our recent work [1] we showed that at low temperatures (below order-disorder transition temperature, T_{ODT}), the slow cooling thermal treatment yields the results which, to some extent, contradict the experimental data and theory.

In particular, the periodicity of the nanostructure below T_{ODT} , and the bridging fraction do not vary with temperature as expected. Despite similar phase behavior, the *mechanical* properties of diblocks and the corresponding A-B-A triblocks differ significantly. This is because the possible arrangements of the triblock chains are different from those of the diblock chains. The triblock chains can form bridges and loops. The triblock chain forms a bridge when its two end blocks are located in two different interfaces separated by a microdomain containing its middle block. By contrast, the end blocks of the chain form a loop if they belong to the same interface. One can control the loops to bridges ratio for a A-B-A triblock melt that orders into lamellar phases to achieve the *desired* mechanical properties.

The slow cooling leads to lamellar spacing and orientation trappings as the temperature decreases. Therefore, we used an alternative method – quenching – where the system is instantaneously cooled down to the required temperature from the athermal state. The results obtained from the quenching method simulation agree well with theory and experiment. Moreover, we noticed an extra low temperature effects which were not observed in the slow cooling scheme, such as an extra peak in specific heat, abrupt decrease of the energy and also corresponding increase of the chain mean squared end-to-end distance and of the periodicity. All these effects were associated with an interfacial ordering from a strongly segregated but still a little diffused lamellar phase to a more strongly segregated phase with a smooth and sharp interface. We described that ordering quantitatively. We also present the results obtained for the symmetric diblock copolymer melts (degree of polymerization $N=16$). Similarly as for the A-B-A triblocks, we performed quenches instead of the slow coolings and recorded the low-temperature effects as for the triblocks. We used a set of four different lattice sizes in order to explore the size effects. The low-temperature interfacial ordering is described quantitatively as for the triblocks [1].

Those effects can be seen regardless of size of the simulation box. In the case of the triblocks (degree of polymerization $N=30$) we reported that the low-temperature ordering at $T^*/N=0.08$. For diblock melts we obtained $T^*/N=0.15$ and it is in agreement with the value for the corresponding triblocks.

In summary, the low-temperature effects can be seen both for the diblocks and the triblocks for a variety of the simulation box sizes, and the temperature scaling behavior for the loops to bridges ratio was obtained. However, there is still an urgent need to perform an off-lattice molecular dynamics simulation to resolve how the underlying lattice affects the low-temperature behavior of block copolymers.

References:

- [1] M. Banaszak, S. Woloszczuk, S. Jurga, T. Pakuła, *J. Chem. Phys.* **119**(21), 11451 (2003).
- [2] M. Banaszak, S. Woloszczuk, T. Pakuła, S. Jurga, *Phys. Rev. E* **66**, 031804 (2002).
- [3] S. Woloszczuk, M. Banaszak, S. Jurga, T. Pakuła, M. Radosz, (unpublished 2004).
- [4] T. Pakula, K. Karatasos, S. H. Anastasiadis, and G. Fytas, *Macromolecules*, **26**, 8463 (1997).
- [5] A. Weyersberg and T. A. Vilgis, *Phys. Rev. E* **48**, 377 (1993).
- [6] L. Leibler, *Macromolecules* **13**, 1602 (1980).

OTHER CONTRIBUTIONS

ON THE EXISTENCE OF NEGATIVE PRESSURE STATES

A. R. Imre

KFKI Atomic Energy Research Institute, H-1525 Budapest, POB 49, Hungary

Some physical quantities can be only positive; others can be either negative or positive. Due to the kinetic-molecular approach - when pressure is introduced as a quantity proportional with particle density - for most people the pressure seems to be in the first group. Although this approach is strictly true only in ideal gases, somehow most of us accepted that pressure cannot be negative. Even when negative pressures were introduced [1], often they were handled as an exotic phenomenon which - due to its metastability - cannot be experimentally seen.

When someone faces with negative pressure in a calculation, the result is often omitted as artefact, because it is a common belief that negative pressure states cannot be physically realized. In reality, for condensed matters, negative pressure exists [2-5]. Real solids are usually not isotropic, therefore it is very difficult to stretch them isotropically along the three axes, i.e. it is difficult to generate a purely diagonal pressure tensor which can be replaced by the scalar thermodynamic pressure. For liquids, the isotropicity is not a problem, but stretching them can be difficult - but not impossible.

Working with materials under negative pressure, one should know the stability limits. All materials will break (for liquids this break means sudden cavitation) applying sufficiently deep negative pressure. This break can happen by gas-phase nucleation or by spinodal decomposition, when - due to the divergence of the compressibility - the material will lose the stability. For liquids this spinodal pressure can be several tens of MPa (for water it is between -200 and -400 MPa), while for solids, it can be with an order of magnitude bigger. Concerning the lifetime of these metastable states, even the liquids - which are more fragile than most solids - can endure deep negative pressure for days. These numbers demonstrate that there is enough "space" to explore below $P=0$.

Recently negative pressure emerged in theories dealing with auxetics [6,7]. Therefore for researchers working with such kind of materials it is important to know the thermodynamics of negative pressure states. In this talk, a brief overview will be given about the experimental and theoretical works on this field.

References:

- [1] L.D. Landau, and E. M. Lifshitz, *Statistical Physics*, Addison-Wesley, Reading, MA, 1958
- [2] D. H. Trevena, *Cavitation and Tension in Liquids*, Adam Hilger, Bristol, 1987
- [3] P. G. Debenedetti, *Metastable Liquids: Concepts and Principles*, Princeton University Press, Princeton, N.J., 1996
- [4] *Liquids Under Negative Pressure* (Eds.: A R. Imre, H. J. Maris and P. R. Williams), Kluwer, Dordrecht, 2002
- [5] A. Imre, K. Martinás, and L. P. N. Rebelo, *J. Non-Equilib. Thermodyn.* **23**, 351 (1998)
- [6] K. W. Wojciechowski, *Molec. Phys. Rep.* **10**, 129 (1995)
- [7] K. W. Wojciechowski, *J. Phys. A: Math. Gen.* **36**, 11765 (2003)

PROPERTIES OF ACOUSTIC PHONONS OF CUBIC AUXETICS

M. Pruchnik¹ and T. Paszkiewicz²

¹ *Institute of Theoretical Physics, Wrocław University, Poland*

² *Institute of Physics, University of Rzeszów, Poland*

Elastic characteristics of crystalline cubic media depend on two parameters. Mechanical stability conditions restrict their values to a triangle on a plane formed by axes corresponding to these parameters. In this triangle there exists a region of auxeticity. For crystalline elastic media belonging to the auxeticity region we study properties of acoustic phonons. In particular, we consider their slowness surfaces and polarization vectors. Novel characteristics of the polarization vectors are introduced.

FE SIMULATION OF THE EFFECT OF POISSON'S RATIO ON INDENTATION RESISTANCE OF MATERIALS

X. J. Ren¹, G. Rothwell¹, C. W. Smith² and K. E. Evans²

¹ School of Engineering, Liverpool John Moores University, Liverpool L3 3AF, UK

² School of Engineering, University of Exeter, Exeter, EX4 4QF, UK

Negative Poisson's ratio materials have many potential advantages over conventional materials as many properties are influenced by the Poisson's ratio, including in-plane stress contraction, shear modulus, bulk modulus, sound and shock absorption and resistance to indentation. Previous experimental studies showed that materials with a Negative Poisson's function have higher indentation resistance independent of their bulk density and modulus. The established relationship between microstructure and Poisson's ratio based on different mechanisms can effectively enable designing materials with Poisson's ratio over a wide spectrum. These beneficial factors will potentially lead to application in fields such as sport or biomedical engineering where protection against indentation loading is of great importance.

Most of the analytical solutions for indentation were limited to linear and homogenous materials, while auxetic materials exhibit a non-linear and highly strain dependent behaviour. In addition, factors such as indenter size, friction, also have significant effect on the indentation process of a material. In this work, indentation resistance of materials with a wide range of Poisson's ratio was investigated using finite element method. The finite element models were validated against known analytical solutions and a parametric study was performed to map the effect of Poisson's ratio. The effect of indenter size, friction between the indenter and the specimen were also systematically investigated and discussed.

References:

- [1] C. W. Smith, R. J. Wooton and K. E. Evans, *Strain dependent densification during indentation in auxetic foams*, Cellular polymer **18**, 79 (1999).
- [2] K. L. Anderson, A. P. Pickles, P. J. Neale and K. E. Evans, *Auxetic polyethylene: The effect of a negative Poisson's ratio on hardness*, Acta Metallurgica et Materialia, **42**, no. 7, 2261 (1994).
- [3] C. W. Smith, J. N. Grima. and K. E. Evans, A novel mechanism for generating auxetic behaviour in reticulated foams: missing rib foam model. Acta Mater. **48**, 4349 (2000).
- [4] X. J. Ren, R. M. Hooper, C. Griffiths and L. J. Henshall, *Indentation size effect (ISE) in single crystal MgO*, Philosophical Magazine A, vol. **82**, no.10 (2002).
- [5] S. P. Timoshenko and J. N. Goodier, *Theory of Elasticity (3rd edition)*, McGraw-Hill Book Company, London (1970).
- [6] K. L. Johnson, *Contact Mechanics*, Cambridge University Press, Cambridge, UK (1985).

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