High performance polymers: Towards intrinsically-auxetic polymers

How to apply

Applicants must email a postgraduate application form (including a 1500 word proposal) to meri@shu.ac.uk by 12 noon on Friday 24 February 2017.

Your application form should clearly indicate the project you are applying for and outline:

a) why you are interested in doing PhD research on this topic
b) how your skills and experience to date (including your undergraduate and/or masters dissertation, if relevant) prepare you to embark on the project
c) any challenges that you foresee in conducting the research and how you might approach or solve them

Where English is not your first language, you must show evidence of English language ability to the following minimum level of proficiency: an overall IELTS score of 7.0 or above, with at least 6.5 in each component or an accepted equivalent. Please note that your test score must be current, i.e. within the last two years.

Please view our eligibility criteria before submitting an application.

Selection process

Successful applicants will be required to attend an interview where you will be asked to talk through your research proposal.

Project details

Director of Studies: Professor Andy Alderson; Second Supervisor: Professor Doug Cleaver

Materials and Engineering Research Institute

External partner: To be confirmed upon application

Project description:

The development of new and improved materials with properties optimised for specific applications is essential to 21st century manufacturing in the UK and globally. One route to developing materials with extreme properties not achievable in conventional materials is to design into them the novel property of auxetic behaviour. Unlike conventional materials which become thinner when stretched, auxetic materials become thicker - they display negative Poisson's ratio behaviour[1].

They are known to display a number of enhanced properties, including vibration damping, novel drape, indentation resistance and fracture toughness. Auxetic polymers have been developed at the macroscale (e.g. foams) and microscale (e.g. microporous polymers and microcellular foams), and naturally-occurring auxetic polymers are known at the nanoscale (e.g. crystalline cellulose). However, an intrinsically auxetic man-made auxetic polymer has thus far not been developed.

The proposed programme is intended to form the first steps in a concerted effort to develop a truly inherent (molecular-level) synthetic auxetic polymer for real-world application. The intention is to identify structure-mechanism combinations with realistic prospects of realising auxetic response in 3D polymeric networks.

The proposal builds on significant prior work by the team at Sheffield Hallam into auxetic structures and mechanisms from the macroscale to the nanoscale. The latter has involved scaling down known macrostructures for theoretical cross-linked polymers[2,3], and understanding natural auxetic inorganic[4,5] and organic crystalline nanostructures[6,7]. In recent work modelling naturally auxetic crystalline cellulose[7], we have successfully identified a single-crystal mechanism giving rise to the observed experimental auxetic response.

We aim to extend our previous work on crystalline cellulose to a fully 3D system having connectivity similar to that achievable in elastomer materials. This will include mono-domain and poly-domain variants.

We will consider firstly structures and mechanisms at a mono-domain level. Analytical and computational models will be developed to yield predictions for mono-domain mechanical properties (Poisson's ratios, Young's and shear moduli). They will allow a first approach to calculating 3D poly-domain properties by employing the well-known Reuss, Voigt and Hill averaging methods.

We will then model a system of domains with each domain employing local homogenised effective properties corresponding to the mono-domain properties. The final and most challenging models will explicitly consider structure in each domain.

The project draws on the strengths within the Materials and Engineering Research Institute from the Auxetic Materials and Materials & Fluid Flow Modelling groups, and is co-funded by a sector leading multinational company providing application focus and exploitation potential.

For further information, please contact Professor Andy Alderson (A.Alderson@shu.ac.uk)

References:

[1] Biomimetics: Designed by Nature - BBC Teach programme

[2] Auxetic Two-dimensional Polymer Networks: An Example of Tailoring Geometry for Specific Mechanical Properties. K.E.Evans, A.Alderson, F.R.Christian. J. Chem. Soc. Faraday Trans. 91(16) (1995) 2671.

[3] Modelling of the Mechanical and Mass Transport Properties of Auxetic Molecular Sieves: An Idealised Organic (Polymeric Honeycomb) Host-Guest System. A.Alderson, P.J.Davies, M.R.Williams, K.E.Evans, K.L.Alderson, J.N.Grima. Molecular Simulation, 31(13) (2005) 897.

[4] Do Zeolites have Negative Poisson's Ratios? J.N.Grima, R.Jackson, A.Alderson, K.E.Evans. Adv. Mater. 12(24) (2000) 1912.

[5] Molecular Origin of Auxetic Behaviour in Tetrahedral Framework Silicates. A.Alderson, K.E.Evans. Phys. Rev. Lett. 89(22) (2002) 225503-1.

[6] Molecular Modelling of Auxetic Behaviour in Cellulose II. Y.T.Yao, K.L.Alderson, A.Alderson. Proceedings of 17th International Conference on Composite Materials (ICCM17) – High Performance Fibre Symposium, Edinburgh 27-31 July 2009, CD-RoM Paper D6.5

[7] Modeling of negative Poisson's ratio (auxetic) crystalline cellulose Iβ. Y.T.Yao, K.L.Alderson, A.Alderson. Cellulose 23 (2016) 3429-3448.