Modelling and Characterisation of Metamaterials with Primitive and Advanced Cellular Structures

Nejc Novak[1], **Matej Vesenjak**[1], **Zoran Ren**[1]

[1] Faculty of Mechanical Engineering, University of Maribor,
Smetanova ul. 17, 2000 Maribor, Slovenia
{n.novak, matej.vesenjak, zoran.ren}@um.si

Abstract. *Modern metamaterials are among the most promising solutions for future applications in engineering, transportation, medicine, sports and many other fields of application. An overview of the development, design, fabrication, computational modelling and characterisation of metamaterials with primitive and advanced cellular structures are described and compared. The optimisation techniques based on validated computational models are developed to design spatially graded cellular metamaterials with enhanced mechanical properties.*

Keywords. Metamaterials, cellular structures, experimental testing, computational simulations, optimisation

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1 Introduction

The rising cost of raw materials, lack of resources, and more stringent policies on sustainable development have resulted in an ever-increasing demand for lightweight and multifunctional materials with improved properties in engineering and other applications. One of the most promising materials for such applications are cellular materials, i.e. materials with internal cellular structure either on nano-, micro-, meso- or macro-scale. Cellular (meta)materials (engineered materials with designed properties) and structures are receiving increased attention in the engineering and scientific community over the past decade due to their low relative density and particular multifunctional properties, making them ideal for modern lightweight engineering and medical applications [1], [2]. Their mechanical and thermal properties make them very suitable for use in automotive, railway, naval, marine and aerospace industry, medicine, as well as in general, lightweight machine design as filters, heat exchangers, isolators, bearings, core material in sandwich structures and as fillers in hollow parts for additional stiffness/support, impact energy absorption and damping [3]. Rapid transition of cellular (meta)materials and structures for industrial applications is affected mainly by expensive fabrication, lack of relevant design guidelines, non-existent practical experience, and general distrust in using new materials. However, new advanced fabrication technologies, e.g. additive manufacturing, enable new trends in the lightweight modern design of cellular structures. This allows outperforming the existing technologies (melt/powder foaming using blowing agents, precursor/replication methods, placeholder method) to produce cellular structures, which do not allow for precise control of the shape, size, and distribution of cells with product predefined topology and morphology settings.

Since cellular structures are increasingly being used, it is critical for the engineering, material and commercial communities to recognise and develop their behaviour under various loading regimes to improve their performance by user-defined (individualised) design. Combining different base materials with the purposely designed internal cellular structure of different morphologies leads to a unique and outstanding combination of multi-material mechanical and thermal properties, tailored by careful design of the cellular structure. New advanced additive manufacturing techniques enable fabrication of the next generation of cellular metamaterials with complex internal cellular structure, adapted to a particular engineering application (including graded porosity) by computational simulations and topological optimisation techniques.

The mechanical behaviour of cellular (meta)materials and structures depends mainly on the relative density (porosity) and the base material, which can be metal or non-metal [1]. The other essential parameters of cellular structures defining their response are morphology (size and shape of the pores, open- or closed-cell structure), topology (regular or irregular pore distribution) and possible filler presence [4], [5]. With careful choice of the geometrical parameters and proper fabrication procedure of cellular structures, it is possible to achieve various mechanical (strength, stiffness, deformation behaviour), damping (phononic band gaps control) and thermal properties (thermal conductivity).

The detailed geometry of the fabricated structures and their influence on mechanical behaviour can be thoroughly evaluated using computed tomography (CT) scanning [6]. The previous research showed that advanced geometrical characterisation significantly depends on the quality of 3D data acquisition. Thus, new and more detailed data on the nano- and micro-scale are needed to build precise 3D digital twins. The 3D digital twins will offer the development of new cellular structures using advanced material engineering methodologies to define individualised geometry and mechanical response of the cellular structures.

In mechanical testing, the compression, tension and bending tests are well-reported and standardised in the literature. At the same time, there is still a lack of data in shear and dynamic testing. The dynamic and impact behaviour of cellular structures was widely studied in the last years using experimental and computational approaches [7]. However, not much work was done on the detailed deformation mechanism analysis of structures with functionally graded porosity [8]. Such a specifically designed internal cellular structure of metamaterials would provide the best desired mechanical response to particular loading conditions [9]. This response can, for example, result in constant deceleration of impacting projectile or constant reaction force on structures under the impact, which is very useful for different applications in safety and defence engineering and crashworthiness. A few successful dynamic experimental tests of auxetic cellular structures have been carried out so far [10], [11]. Simultaneously, computer simulations have been used to analyse the response of various cellular structures under dynamic loading, but only a few have been validated with the experiments [11].

The micro-architected cellular structures and micro- and nano- latices with unit cell size below 1 μm were developed recently [12], [13]. Periodic phononic metamaterials comparable to the wavelength of optical or acoustic waves were the first drivers towards the miniaturisation of cellular structures to control the band gaps. Recently, micro- and nano-lattices were also simultaneously designed to enable unique scale-independent properties such as tailorable stiffness, deformability, thermal expansion, and auxetic behaviour. The detailed analysis of mechanical behaviour at different strain rates, optimisation of the fabrication procedure and geometry, and the introduction of biodegradation and biocompatibility in micro- and nano-lattices is still very limited. The multiscale cellular structures are also a promising route toward developing life-lasting implants, stents and other medical devices [14].

As it can be concluded from the above short state-of-the-art review, there is still a lack of research in detailed geometry characterisation and the consequent development of digital twins, which will offer the development of new geometries and optimised fabrication procedures. The research on the mechanical testing and subsequent computational simulations of the multiscale multi-material lattices and the high strain rate and shear testing of cellular structures is also minimal. The work done at the University of Maribor on bridging the gap in the metamaterials research is presented.

2 Geometry and fabrication of (meta)materials

The (meta)materials are divided into groups in the following section depending on their topology and manufacturing procedure. Some of them are shown in Figure 1, where the development from primitive to advanced geometries through time is presented.

Figure 1. Research of cellular metamaterials at the University of Maribor in recent years: from primitive to advanced cellular geometry

2.1 Open-cell foams

Open-cell foam represents an interconnected structure of cells. Polymeric open-cell foam can be easily compressed and then naturally recover to its original shape. As a result, open-cell foam is most widely known for its use in the furniture industry as sofa cushion foam, foam mattresses, car seats and acoustic and soundproofing. The metal open-cell foams used are mainly produced using the investment casting method. The starting point is a porous polymer precursor. The pores are filled with a refractory slurry, dried and burnt. During combustion, the precursor pyrolysis, while the slurry hardens and forms the mould for the subsequent investment casting of the metallic matrix. The final step is removing the moulding material, which results in a porous metallic geometry very similar to the polymer precursor [5].

The mechanical properties of metal open-cell materials primarily depend on the properties of the base material, morphology and topology of the cells. The influence of the base material on the properties of metal foams is well studied. There are many empirically established relationships linking the properties of the base material and morphology with the properties of the cellular material. Metals and alloys used for metal foams must have a low density to maintain the advantage of low relative density over conventional solid materials. For this reason, the most commonly used metals for cellular materials are aluminium, magnesium, titanium and their alloys [15].

The influence of cell morphology on the mechanical properties of regular and irregular open-cell materials has been investigated by many authors using the representative unit cell. It was assumed that the behaviour of the cell material could be described well enough with a single, geometrically uniform cell. Since the cell geometry of fabricated open-cell foams differs from the geometric regularity, many authors have also investigated the cell morphology of

fabricated foams [16]. The mechanical behaviour of the open-cell foam can be further increased by introducing the polymer filler to the cellular structures [17]. The open-cell foams can also be used as a filler for foam-filled tubes [18].

2.2 Closed-cell foams

Closed-cell foam consists of interlocking micro- and macroscopic cells sealed shut, preventing air or water from passing through. This type of foam is stiffer and water-resistant, making it highly suited to shock absorption and thermal insulation. The closed-cell aluminium foam is produced using the powder metallurgical method [19], which consists of placing extruded, foamable precursor in a stainless steel mould in a preheated oven. The mould cavity is then filled by foaming the precursor, made of aluminium, silicon and titanium hydride. The mould with moulded foam is removed from the oven and cooled to room temperature. The aluminium foam is then removed from the mould made of carbon steel and cut lengthwise to prepare the specimens. The mechanical behaviour of closed-cell aluminium foams has been thoroughly characterised under free and laterally constrained compression loading conditions [20]. The same foams were also introduced into tubes (*ex-situ* foam-filled tubes), which enhanced the mechanical response. Powder metallurgical foam production also allows the production of closed-cell foams inside the tubes (*in-situ* foam-filled tubes) to achieve increased stiffness through better bonding between the foam filler and the outer tube [21].

2.3 UniPore structure

The unidirectional UniPore structure with longitudinal pores initially consists of an outer tube and thin-walled inner tubes, which are welded together with an explosion welding technique [22]. Before manufacture, the outer tube is tightly packed with inner tubes of a much smaller diameter over the entire length of the sample. The structure of the porous UniPore metal produced by this method has a uniform porous cross-section in the longitudinal direction, with the pore length being limited only by the size of the samples.

The inner tubes of different thicknesses with constant outer tube thickness were used to produce samples with three different porosities. The moderate welding condition necessary for the successful interface formation is not fulfilled in some regions between the inner pipes due to different collision angles of the pipes because of their round outer interface. This was also be studied with computational simulations [23].

A new production method for UniPore structures was thus proposed [24]. It is based on rolling cheap thin metal foil with acrylic spacer bars positioned on a surface and subsequent explosive compaction. As soon as the thin film between the spacers is uniformly accelerated, the welding condition associated with the collision angle is considered stable, similar to conventional explosive welding. The manufacturing process of newly developed unidirectional metallic copper is similar to the one used for original UniPore cellular structures. Thin foils of other metallic materials can also be applied. It should be noted that the external

dimensions, the size of the pores, the thickness of the internal walls and the porosity can be easily adapted to individual application requirements.

2.4 Advanced pore morphology (APM) foam

Advanced pore morphology (APM) foam with a hybrid cellular structure was developed in Germany at the Fraunhofer IFAM, Bremen. APM foam elements consist of sphere-like interconnected closed-cell porous structures within solid outer skin. The manufacturing procedure consists of powder compaction and rolling of AlSi7 alloy with TiH2 foaming agent to obtain expandable precursor material. The precursor material is cut into small volumes (granules), which are then expanded into spherical foam elements due to the heat reaction of the TiH2 foaming agent in a continuous belt furnace. The internal structure of APM was evaluated [6], [25]. The APM elements were also used as a filler material for foam-filled tubes [26], [27].

2.5 Predesigned structures

Advanced fabrication techniques, such as additive manufacturing, allow producing predesigned structures. Three-dimensional auxetic cellular structures [28] presented here are built up from inverted tetrapods [11] and chiral auxetic structures [29]. The unit cells of inverted tetrapods are stacked in layers and then into the layered three-dimensional auxetic structure [30]. The auxetic cellular structures were constructed as CAD models and produced using the selective electron beam melting method (SEBM) from the Ti-6Al-4V alloy. The shape of the chiral auxetic structure unit cell corresponds to the 10th eigenmode of the regular cubic unit cell, which was presented in [31]. The mechanical properties can be further enhanced with the introduction of the polymeric filler [32].

High potential in many engineering applications also represents the periodic cellular materials, especially triply periodic minimal surfaces (TPMS). TPMS are complex 3-D topologies that locally minimise surface area for a given boundary and can be repeated periodically in three perpendicular directions [33]. These surfaces split the space into two or more interlocked domains, where each domain is a single connected and infinite component with no enfolded voids. Due to their novel topological features, TPMS have been employed in many engineering disciplines, such as tissue engineering [33], and structural engineering [34]. They also have optimal thermal and electrical conductivity [35] and optimised fluid permeability [35].

3 Design and characterisation

The main focus of the computational characterisation of the metamaterials is in the development of reliable numerical models, which have to be validated with the experimental tests. Different simplifications can be adopted to the computational models based on the geometry and planned further use.

3.1 Experimental testing

Most of the experimental tests were done in compression, which shows a typical mechanical behaviour with the initial elastic region, followed by the plateau and densification.

The behaviour of closed-cell foams under various loading conditions has been studied in detail [40] using micro-computer tomography (μCT) to track changes in the internal structure during the deformation of closed-cell aluminium foam [6]. Different closed-cell foams were tested under compressive and bending loading [41]–[45].

The compression [26] and bending [27] tests of APM and APM filled tubes were also performed. Besides this, the change in the geometry of the APM during loading was analysed in [46].

The influence of the loading velocity on the mechanical behaviour of closed-cell aluminium foams [47] was analysed with the Split Hopkinson Pressure Bar (SHPB) apparatus. The compression behaviour of foams made of aluminium alloys at high strain rates has also been investigated and discussed in [7], [48]. High strain rate testing using a powder gun was done for open-cell foams [49], closed-cell foams [50] and auxetic structures [11], [51]. Three-point bending tests were also used for the evaluation of the bending response of foam-filled tubes [27], [42], [43]. The shear testing of open-cell foams [52] and auxetic cellular structures [53] was also done recently.

3.2 Homogenised computational models

In the case of closed-cell foams, the simple computational model with the applied homogenised material model (crushable foam) with volumetric hardening was built in Abaqus finite element software, where the explicit solver was used for analysis. Due to the axial symmetry of the specimens, axisymmetric boundary conditions could be applied in the computational model. The crushable foam constitutive model parameters were determined with the optimisation algorithm, whereby first, the quasi-static (Q-S) experiment and the computational responses were compared (Figure 2). After optimising the material parameters, the same material model was used for the high strain rate (HSR) load. Good agreement can be observed for both quasi-static and HSR tests. The agreement between the experimental and computational responses is very good for both analysed strain rates (Figure 2). The discrepancy can only be observed at lower strains of the HSR response, where only the first stress peak could not be observed in the computational model due to the initial boundary conditions. The stress peak is a consequence of the collision in the experiments and represents a typical reaction of the structures during the initial phase of the impact but does not influence the global behaviour afterwards [11].

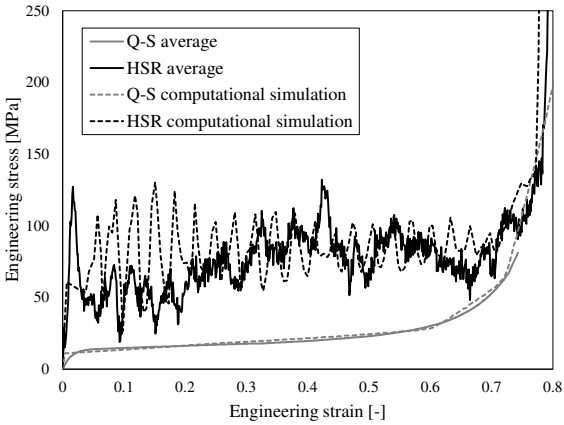

Figure 2. Engineering stress-strain relationship of closed cell foam under quasi-static (Q-S) and high strain rate (HSR) loading conditions.

The deformation behaviour under quasi-static and HSR loading conditions is shown in Fig 3. Under quasi-static load, a uniform deformation of the sample can be observed. The change in the deformation mode can be observed in the case of HSR loading, where the deformation is localised at the impact surface between the load plate and the specimen.

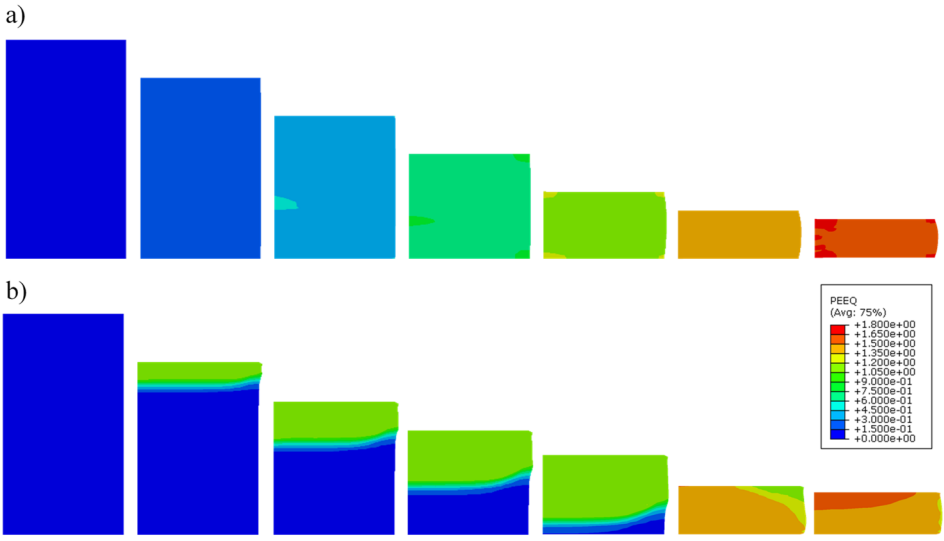

Figure 3. Evolution of the equivalent plastic strain (PEEQ) during the quasi-static (a) and high strain rate (b) deformation response of closed-cell foam modelled with homogenised computational model.

3.3 Discrete computational models

The discrete computational models offer a more precise analysis of the deformation behaviour of the metamaterials but at higher computational costs than the homogenised models. The strut based cellular structure, such as open-cell foams and auxetic structures, are mostly modelled with the beam finite elements [8], [36], [37].

The computational models of TPMS lattices are generated using the shell finite elements using the MSLattice code [38] to generate the fundamental lattice geometry of TMPS samples [40]. Meshing was performed by the PrePoMax software [45], and the boundary conditions were defined in the LS-PrePost software. The manufacturing imperfections resulting in plate thickness variation were also analysed [41] and were considered indirectly through the used material parameters determined by inverse parametric computational simulations.

The computational results of the constituent TMPS lattices were compared in terms of mechanical response (stress-strain relationships) and deformation behaviour to quasi-static experimental data from [39] for each analysed geometry and relative density. The computational models' deformation behaviour was validated with experimental observations recorded by HD video camera. The experimental and computational deformation behaviour of diamond TPMS lattices with different relative densities are shown in Figure 4. The overall response is quite comparable.

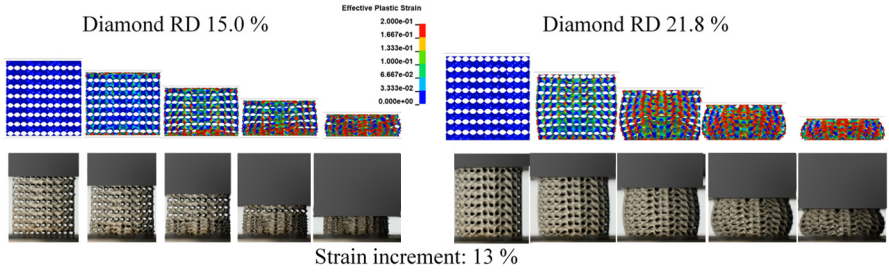

Figure 4. Comparison between the computational and experimental results in case of TPMS structures modelled with shell finite elements.

The volume finite elements were also used to discretise the open-cell foams. The correct geometric representation of fabricated aluminium open-cell foam samples requires a sufficiently high resolution of the µCT scan to capture geometric details and allow for accurate segmentation of the metallic phase. Figure 5 shows the deformation of the open-cell foam with contours representing von Mises stresses during loading. A gradual and uniform deformation of the foam is observed.

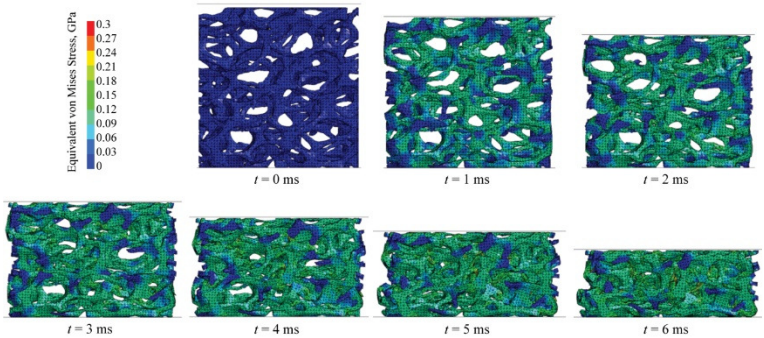

Figure 5. The deformation behaviour of open-cell foam modeled with volume finite elements.

4 Optimisation and development of new geometries

The validated computational models offer the possibility for further development and optimisation of new metamaterials.

New auxetic geometries were developed using a topology optimisation [54]. A 2D plane stress state simplification was used to model the auxetic structure. Only one cell of the periodic structure was selected as the domain for the multi-objective optimisation. One-quarter of this cell was used in the computational model to simplify the procedure further. In contrast, the rest of the cell was replaced by applying appropriate double symmetry boundary conditions. This simplification was introduced since double symmetry can be found in many existing auxetic structures such as re-entrant hexagons, symmetric chiral structures and sinusoidal ligament structures.

TPMS lattices are materials designed mathematically. Therefore, the advanced fabrication methods offer the fabrication of graded a hybrid structure, where different geometries can be combined. A graded or hybrid structure can enhance its topology to exhibit more advantageous and desired properties. A finite element computational model was developed in LS-DYNA to capture the mechanical properties of additively manufactured uniform TPMS-based lattices made of stainless steel 316L tested under quasi-static and dynamic loading conditions. The validated computational model was used to predict the mechanical behaviour of the newly developed hybrid TPMS cellular lattice with spatially varying gyroid and diamond cells in the longitudinal and radial direction (Figure 6). The new hybrid lattices were fabricated and mechanically tested, where good agreement between experimental and computational results was achieved [55].

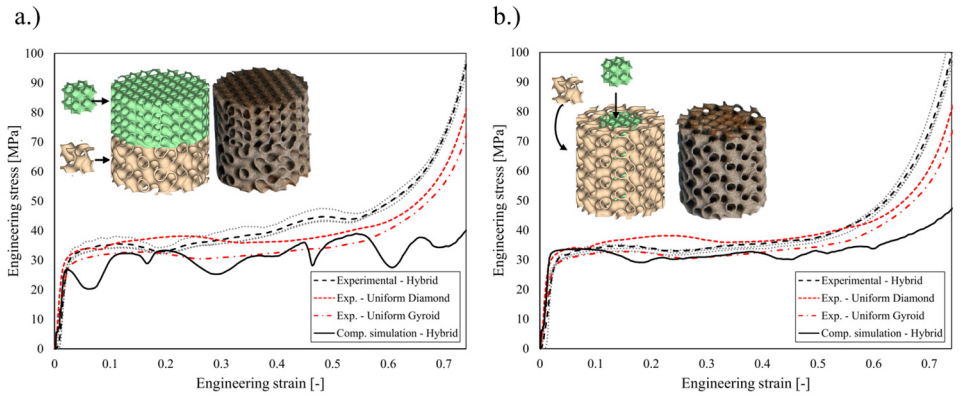

Figure 6. Comparison between the computational and experimental results for linear (a) and radial (b) hybrid TPMS lattices

Novel three-dimensional (3D) axisymmetric chiral structures with negative and zero Poisson's ratios were developed based on the existing 3D conventional chiral unit cell [37], [56]. The conventional tetra-chiral unit cell is mapped to the axisymmetric space to form the new 3D axisymmetric chiral structure. The structures are fabricated using additive manufacturing technology and experimentally tested under compression loading conditions. The computational model of axisymmetric chiral structures is developed and validated using the experimental data. The computational model was then used to evaluate the new axisymmetric chiral structures with graded cell structures. The newly developed axisymmetric structures show enhanced mechanical properties compared to the existing 3D chiral structures.

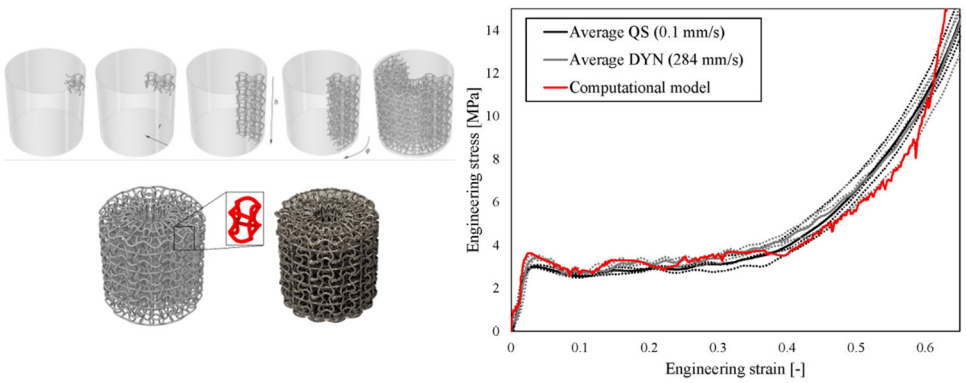

Figure 7. Design of the axisymmetric auxetic structure (left) and comparison between the computational and experimental results (right) under quasi-static (QS) and dynamic (DYN) loading conditions

5 Conclusions and outlook

The design, fabrication and mechanical behaviour of various cellular structures, from quasi-static to high strain rate loading, is presented. The experimental results of these structures under compression loading are compared to the specific energy absorption (SEA) capacity up to 50 % strain in Figure 8. The darker shading colours in Figure 8 correspond to lower specimen porosity in each analysed group of cellular structures, while lighted shading denotes higher porosity specimens. It can be observed that porosity and base material strongly influence the SEA capacity. Structures with lower porosity can absorb more mechanical energy through deformation than structures with higher porosity that exhibit lower stiffness. The same conclusions can also be reached for base materials, where materials with higher Young's modulus show higher SEA capacity. The best consistent SEA at 50 % strain can be observed for closed-cell foams, TPMS structures and UniPore structures. In UniPore structures, densification already appears at 50 % strain (Figure 8) and shows SEA is thus the total SEA for this type of structure. Closed-cell foams (Figure 8) and other analysed cellular structures densify at much higher strains, contributing to higher total SEA capacity.

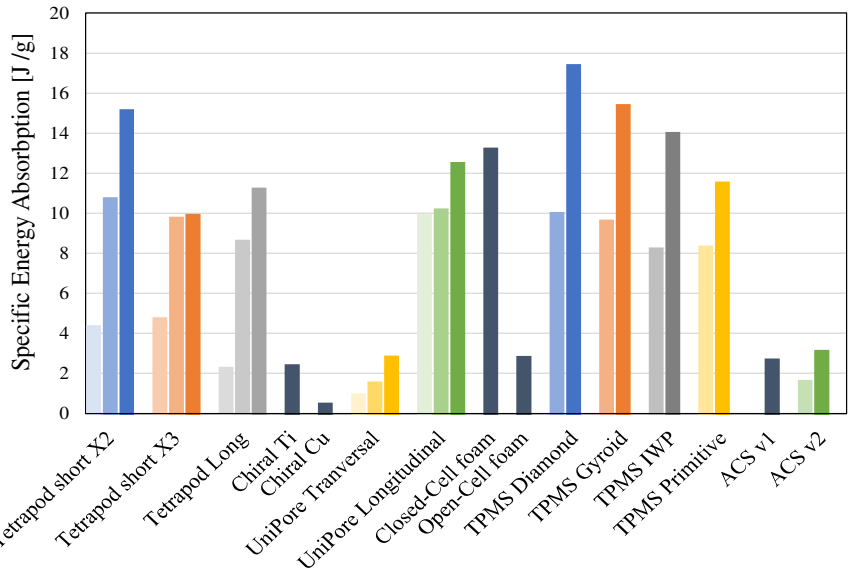

Figure 8. Comparison between the computational and experimental results

The computational simulations are an excellent tool for preliminary evaluation of new cellular designs and a better understanding of the deformation behaviour of various cellular structures. Different approaches are presented in this article, from simpler and fast homogenised computational models to advanced detailed and time-consuming processes, where a whole cellular structure is modelled with volume finite elements. A further improvement of computational models is imminent with the development of computational power and software capabilities, which will enable mesoscale modelling approaches to consider also

influences of fabrication defects. Consequently, it leads to more precise virtual prediction capabilities of cellular metamaterial deformation behaviour and better possibilities for optimisation of their mechanical response.

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