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Optimal Design and Additive Manufacturing of Polymeric Metamaterials for Energy Absorption and Impact Mitigation

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Abstract. Architected metamaterials fabricated by additive manufacturing offer deterministic geometries and tunable mechanical properties that can outperform conventional foams in energy absorption and impact mitigation. In this work, origami honeycomb and plate-lattice metamaterial concepts are unified within a common, quantitatively characterised metamaterial. An optimization-based design approach is employed to maximise absorbed energy while keeping the peak stress below a predefined threshold, using metamaterial geometric parameters as design variables. The objective function is evaluated through post-processing of Abaqus compression simulations on automatically generated designs. Owing to the high computational cost, the optimisation is performed using an evolutionary algorithm with a limited number of evaluations, yielding a best-performing design rather than a global optimum. Despite this limitation, the results elucidate the critical roles of buckling in limiting initial peak stress and of contact in enhancing post-peak energy absorption, and they highlight the significant potential for further performance gains through expanded design space exploration.

Introduction

Recent advances in architected ("meta") materials have enabled cellular structures with deterministic geometries and tunable mechanical properties that outperform conventional stochastic foams in energy absorption and impact mitigation. Townsend et al. [1] developed origami honeycombs with fold geometries designed to tailor stress–strain responses and energy absorption. These metamaterials, fabricated from thermoplastic polyurethane (TPU) via fused filament fabrication (FFF), combine the elastic recoverability of TPU with the geometric freedom of additive manufacturing. More recently, Smith et al. [2] introduced tunable plate-lattice metamaterials for impact mitigation, also manufactured by FFF using TPU, achieving up to an order-of-magnitude higher energy absorption than conventional foams at comparable peak stresses. These studies form the basis of the optimal design approach proposed here.

In this work, we assimilate Townsend et al.'s origami honeycombs and Smith et al.'s plate-lattice metamaterials into a common, quantitatively characterised material framework. We then apply an optimization-based metamaterial design approach [3], treating the parameters that characterise the metamaterial as design variables. The objective is to maximise absorbed energy while constraining the peak stress below an admissible threshold for impact mitigation. Objective evaluations are obtained by post-processing Abaqus compression simulations of automatically generated designs.

The optimisation problem is solved using an evolutionary algorithm, with the number of objective function evaluations limited to a few tens due to the high licensing cost of Abaqus. Consequently, we report a best design—rather than a true optimum, given the limited exploration of the design space. Despite this limitation, comparison among evaluated designs clearly reveals the role of buckling in limiting the initial peak stress and the contribution of contact to enhancing post-peak energy absorption. The results further indicate that substantial improvements in energy absorption and impact mitigation may be achieved by exploring a richer design space once the licensing constraint is removed.

Parametrisation

The current work aims to apply the optimization-based metamaterial design (OMD) approach to optimize the performance of metamaterials for energy absorption and impact mitigation. In OMD, the objective function characterises the performance to be optimised, and the design variables define the metamaterial. The first step is the parametrisation of the considered metamaterials, in order to define the design space.

The currently studied metamaterials are based on the origami honeycombs proposed by Townsend et al. [1] and the place-lattice metamaterials proposed by Smith et al [2]. Figure 1 shows an origami honeycomb [1], which is characterised by the unit cell side b, the wall thickness t, the number n_z of cells in the z (loading) direction, the number n_x of cells in the x and y directions, and the aspect ratio a, that equals 1 when the unit cell is a prismatic tube, and reduces as the fold angle increases. Ref. [1] evaluated the energy absorption performance of these origami honeycombs for several values of n_z and a; which played the role of design variables for energy absorption optimization in their work.

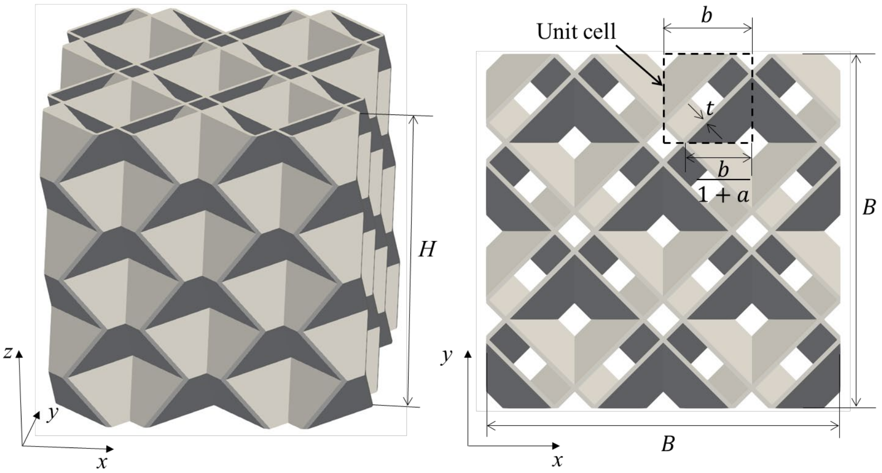

Fig. 1. Origami honeycomb and its topological parameters.

Figure 2 shows a plate-lattice metamaterial [2], which is defined by the size w and height h of the unit cell, the wall thickness t, and the geometric prebuckling parameter p, which is equal to zero when the unit cell is a prismatic tube and increase with the folding angle, and the number of cells in the loading direction and across it, n_z and n_x, as before. Ref. [2] evaluated the energy absorption efficiency for several values of p and the plate-lattice density ρ. Since they kept w, h, t, n_z and n_x fixed, p is the only variable in the definition of ρ; so p can be seen as the only design variable in their work. Note that they allowed p to change in the loading direction, so p is not one scalar but a set of n_z scalar design variables.

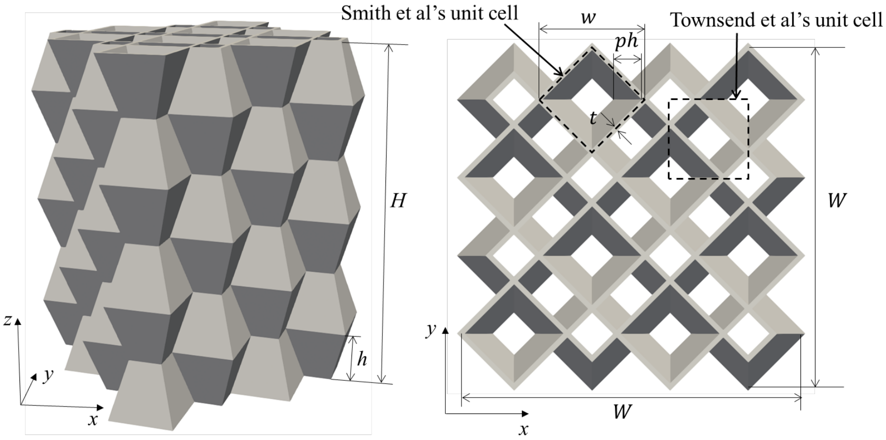

Fig. 2. Plate-lattice metamaterial and its topological parameters.

However, beyond their particular denominations, Townsend et al’s origami honeycombs [1] and Smith et al’s plate-lattice metamaterials [2] just define different unit cells of the same periodic metamaterial, as shown to the right in Figure 2. Their geometrical parameters related by:

$$p = \frac{1-a}{1+a}\frac{b}{h}, \; w = \frac{2}{1+a}b \tag{1}$$

Therefore, we adopt the unit cell as defined by Smith et al [2], since it is easier to build using the drawing and meshing tools provided by Abaqus and Salome_Meca, which are the finite element packages used in this work. Therefore, any sample of the current metamaterial with given dimensions $W \times W \times H$ is characterized by the following design variables: 1) the prebuckling parameter p, 2) the number n_z of cells or folds in z direction, 3) the number n_x of cells in the x and y directions, 4) the wall thickness t.

This geometrical parametrisation was implemented via two alternative Python scripts, one called *XtoGeoAbaqus.py* made for running under the Abaqus shell, the other called *XtoGeoSM.py* that runs under the Salome_Meca shell. Each script takes the geometrical design variables as input and generates the geometry of the corresponding design in STL (stereolithography) format, which is a common file type for slicer software for 3D printing. Using either of these scripts, a large series of designs can be automatically generated in the search of the optimal design. Figure 3 shows some of the generated designs.

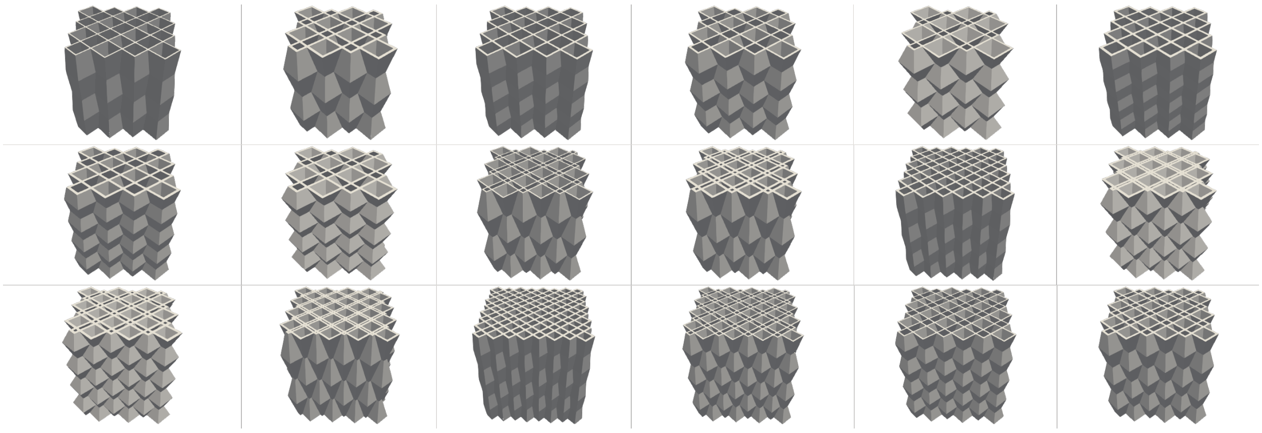

Fig. 3. Parameterised metamaterial samples.

Fused filament fabrication (FFF) using thermoplastic polyurethane (TPU) is a common technique for the additive manufacturing of these metamaterials. Townsend et al [1] and Smith et al [2] modelled the TPU material as a Mooney-Rivlin hyperelastic material and an Ogden-Prony viscoelastic material, respectively. Smith et al [2] based their choice of TPU grade on the need of a material being soft enough to enable relatively low-force characterization experiments, and stiff enough to allow robust, repeatable fabrication of many samples with high yield. The choice of material, in particular its hardness, affects the metamaterial’s response. Hence, a new design variable, say m, can be added to define the material. In the current approach, the material properties are assumed to be uniform and independent of the additive manufacturing conditions.

In summary, any design of the current metamaterial is fully described by the following set of design variables:

$$X = [p, t, n_x, n_z, m] \tag{2}$$

where p and t are real number variables, n_x and n_z are integer variables and m is a categorical variable. The set X belongs to the mixed-variable (discrete-continuous) design space D, where each variable is properly bounded. Further, Smith et al [2] allowed p to vary in the z direction, making p not one but a set of parameters. Given the freedom offered by additive manufacturing, not only prebuckling but also thickness and cell size could be variables inside the sample, enriching the design space.

Characterisation of the energy absorption and impact mitigation performance

We characterise the mechanical response to energy absorption and impact mitigation by the relation between the stress $\boldsymbol{\sigma}$ and the strain $\boldsymbol{\varepsilon}$ under compression loading. We consider bulk measures of $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$, defining $\boldsymbol{\varepsilon}$ as the ratio between the magnitude $\boldsymbol{\Delta H}$ of the applied compressive displacement and the initial height $\boldsymbol{H}$ of the sample, and $\boldsymbol{\sigma}$ as the ratio between the magnitude $\boldsymbol{R}$ of the resultant of reactions at $\boldsymbol{z = 0}$ and the initial area $\boldsymbol{W^2}$ of the cross section. Note that both $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are magnitudes, i.e., $\boldsymbol{\sigma > 0}$ and $\boldsymbol{\varepsilon > 0}$.

The energy absorbed per unit volume by the sample when it is compressed up to the strain $\boldsymbol{\varepsilon_{end}}$ is:

$$A(\varepsilon_{end}) = \int_0^{\varepsilon_{end}} \sigma(\varepsilon)d\varepsilon \tag{3}$$

Townsend et al [1] and Smith et al [2] characterised the performance of the current metamaterials using the energy absorption efficiency:

$$E^*(\varepsilon_{end}) = \frac{\int_0^{\varepsilon_{end}} \sigma(\varepsilon)d\varepsilon}{P(\varepsilon_{end})} \tag{4}$$

where P is the peak stress:

$$P(\varepsilon_{end}) = \max_{\varepsilon \leq \varepsilon_{end}} \sigma(\varepsilon) \tag{5}$$

Figure 4 shows the $\sigma(\varepsilon)$ curve for a metamaterial sample with $W = 38.4$ mm, $H = 38.4$ mm, prebuckling $p = 0.4$, $n_x = 4$ cells in x and y directions, $n_z = 6$ cells in z direction, wall thickness $t = 0.6$ mm, compressed at 36 mm/s (i.e., 0.75/s strain rate) in z direction, as obtained using Abaqus explicit module, adopting the Ogden hyperelastic material model as calibrated by Smith et al [2]. Let us note Smith's material model also include viscous terms, which are neglected in the current study. Smith et al [2] performed repeated loading-unloading tests, allowing the samples to recover a minimum of 1000 s such that viscoelastic effects are relevant [2]. Then, they used a Prony series model to capture these time-dependent effects. On the other hand, Townsend et al [1] allowed a much shorter recovery between tests, neglecting viscoelastic effects. Being the current study restricted to only one loading cycle, we neglect viscoelastic effects following Townsend et al [1].

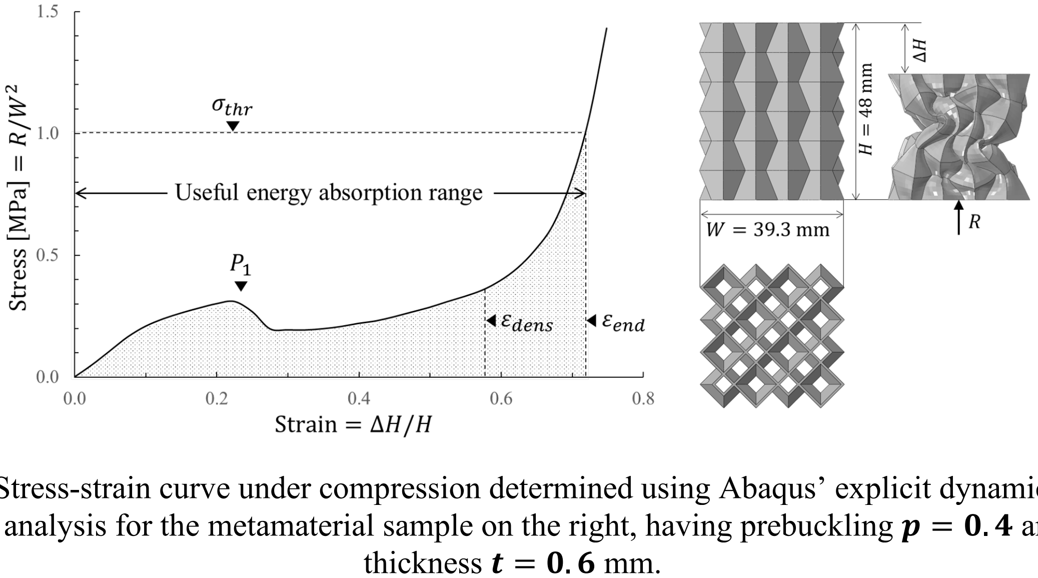

Fig. 4. Stress-strain curve under compression determined using Abaqus' explicit dynamic finite element analysis for the metamaterial sample on the right, having prebuckling $\boldsymbol{p = 0.4}$ and wall thickness $\boldsymbol{t = 0.6}$ mm.

This curve exhibits common features of the response of the current energy-absorbing metamaterials. The initial stress peak P_1, corresponding to the onset of structural instability, is subsequently attenuated by buckling. After this peak, the load-bearing capacity decreases as buckling progresses until the onset of contact between different faces or even self-contact in a largely deformed face. Beyond this point, the bearing capacity increases again due to progressive compaction, reaching the so-called densification strain ε_{dens}, after which there is a sharp increase in the slope of the $\sigma(\varepsilon)$ curve. Townsend et al. [1] reported ε_{dens} to vary between 0.55 to 0.60 for origami honeycombs with aspect ratio a varying between 0.6 and 0.9. Let us note that there is a large dispersion in the definition of the densification strain [7]; unfortunately, Townsend et al. [1] did not specify which one they used.

The densification strain ε_{dens} is usually considered to be the upper limit of the useful energy absorption range, named ε_{end}, as it is the case for the metamaterials of Townsend et al [1] and Smith et al [2]. However, for impact mitigation problems, the upper limit of the useful energy absorption range should actually be defined by the injury threshold level σ_{thr} [6]. To adopt $\varepsilon_{end} = \varepsilon_{dens}$ may lead to either an underestimation of the energy absorption efficiency (if $P(\varepsilon_{dens}) < \sigma_{thr}$) or inadmissible responses (if $P(\varepsilon_{dens}) > \sigma_{thr}$). To avoid these cases, and the uncertainty in the definition of ε_{dens} as well [7], we define the upper strain limit ε_{end} by the following relation

$$P(\varepsilon_{end}) = \sigma_{thr} \tag{6}$$

Optimisation of the energy absorption and impact mitigation performance

The application of the optimization-based metamaterial design (OMD) approach [3] to the metamaterials and objectives considered by Townsend et al [1] and Smith et al [2] gives rise to the following mathematical optimization problem:

$$\max_{X \in D} \frac{\int_0^{\varepsilon_{end}} \sigma(\varepsilon) d\varepsilon}{P(\varepsilon_{end})} \tag{7}$$

having the energy absorption efficiency E^* as the objective function. If ε_{end} is not defined by Eq. (6) but prescribed, the following non-linear inequality constraint must be considered:

$$P(\varepsilon_{end}) \leq \sigma_{thr} \tag{8}$$

In this work, having defined ε_{end} by Eq. (6), we prefer to solve a simpler optimization problem

$$\max_{X \in D} \int_0^{\varepsilon_{end}} \sigma(\varepsilon) d\varepsilon \tag{9}$$

i.e., considering the energy absorption per unit volume $A(\varepsilon_{end})$ as the objective function.

The objective function depends on the design variables X via the $\sigma(\varepsilon)$ relationship. Embodying the Python script *XtoGeo.py* that takes the geometrical design variables and builds the domain of analysis (discussed in the previous section), we coded the Python script *XtoFE.py* that takes as input all the design variables and gives as output the finite element (FE) model for Abaqus. Note that only Abaqus is kept henceforth, since Salome_Meca solutions diverge as soon as the contact onset is attained.

Running the FE model with Abaqus gives the $\sigma(\varepsilon)$ curve as result. A new Python script called *Fitness.py* takes the $\sigma(\varepsilon)$ curve as input, computes ε_{end} for the given σ_{thr}, and finally the objective function $A(\varepsilon_{end})$.

Gradient-based algorithms were preferred in the previous OMD applications developed by Fachinotti and collaborators, e.g. [3]. Here, without an explicit analytical relationship between the objective function and the design variables, we must compute the gradient numerically, which is prohibitively expensive; for instance, the determination of the $\sigma(\varepsilon)$ curve in Figure 4 took more than 12 hours. Furthermore, the nature of Abaqus' explicit dynamic analysis with automatic time stepping introduces discontinuities in the dependence of the objective function on the design variables. Therefore, we solve the current optimisation problem, Eq. (9), using evolutionary algorithms [13]. Figure 5 shows the integrated computational workflow for the optimization-based design of these energy-absorbing metamaterials. This is a straightforward adaptation of the workflow developed by the authors for the optimization of the microstructure in 3D printed duplex steels [9].

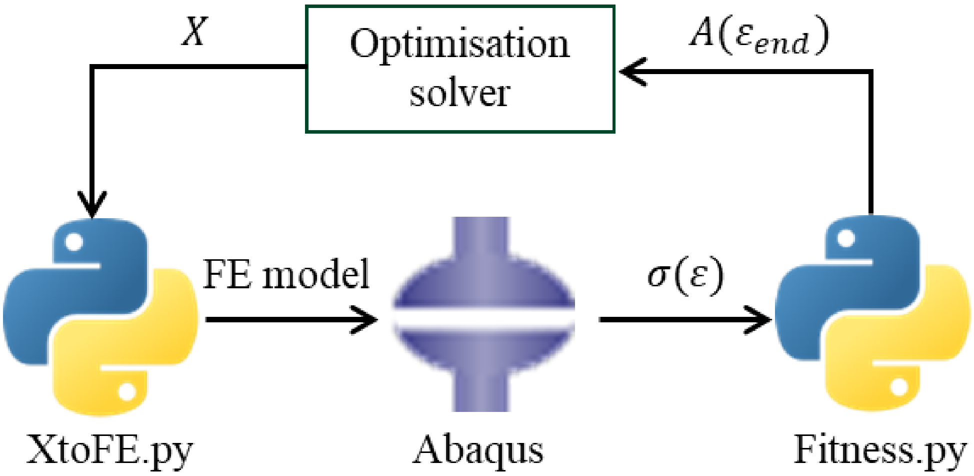

Fig. 5. Workflow for energy absorption optimisation in metamaterials.

Results

The stress-strain response of the current metamaterials is obtained using the commercial finite element software Abaqus. The material behaviour is modelled using the Ogden hyperelastic law calibrated by Smith et al [2]. Regardless of the loading rate, the use of Abaqus' explicit dynamic solver is mandatory, since, unlike the static solver, it includes the general contact model. This contact model does not require to explicitly define every possible contacting pair, which is impractical (even impossible) in presence of folding, buckling, and large deformation problems where parts may touch unexpectedly and self-contact occur. Given its robustness, it has been chosen by Townsend et al [1] and Smith et al [2]. Following these authors, we also assume a Coulomb-type friction between all contact surfaces. We adopt a sliding coefficient of friction equal to 0.75, value proposed by Smith et al [2] to imitate real-world conditions of contact between plastics, other elastomers, or flesh.

The lack of such a robust contact solver in Salome_Meca precludes the use of this free and open-source software for the current purposes. On the other hand, the high cost of the Abaqus license for the current, highly time-consuming problems, obliges us to limit the number of iterations when solving the optimisation solution problem to 20, less than those that are typically needed to satisfy a convergence criterion.

Other simplifications for limiting the computational cost concern the design variables. We will consider only one material. Hence, only the geometrical design variables are kept. Further, the categorical design variables are allowed to take just a few levels: two for the wall thickness t (0.6 and 0.8 mm), and two for the number of folds n_z (6 and 8). A larger freedom is allowed for the prebuckling parameter ($0 \leq p \leq 0.8$), but a unique value is adopted to the whole structure instead of changing across the loading direction, as proposed by Smith et al [2].

We assume $\sigma_{thr} = 1$ MPa, which gives a reasonable security margin to keep the peak transmitted stress below 1.5 MPa as required for head health applications [6].

Figure 6 shows some of the designs evaluated in the optimisation process. The best design has prebuckling $p = 0.6$, wall thickness $t = 0.6$ mm, and $n_z = 6$ folds in the compression direction.

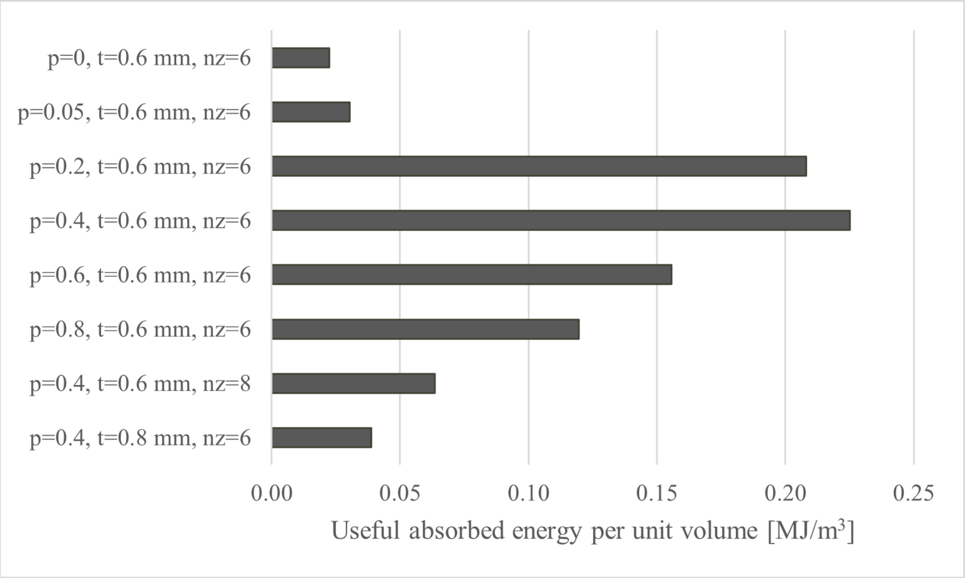

Fig. 6. Absorbed energy per unit volume under compression up to the stress threshold (1 MPa) for different values of prebuckling (p), wall thickness (t), and folds in the loading direction (nz).

Figure 7 shows the $\sigma(\varepsilon)$ curves for some designs, highlighting the crucial role of the design variables in the energy absorption performance. Low prebuckling may lead to an excessive stress peak, above the prescribed threshold σ_{thr}, considerably shortening the useful energy absorption range. Large prebuckling can make the metamaterial excessively soft, lowering the energy absorption even if the useful range is large. Increasing the wall thickness makes the metamaterial stiffer, showing a first stress peak that may exceed σ_{thr}. Compared to the best design, a design having the same prebuckling (0.6) and wall thickness (0.6 mm) but more folds in the loading direction (8 instead of 6) was stiffer, showing a first stress peak that exceeds σ_{thr}. More designs with varying n_z are needed to explain the cause of this difference.

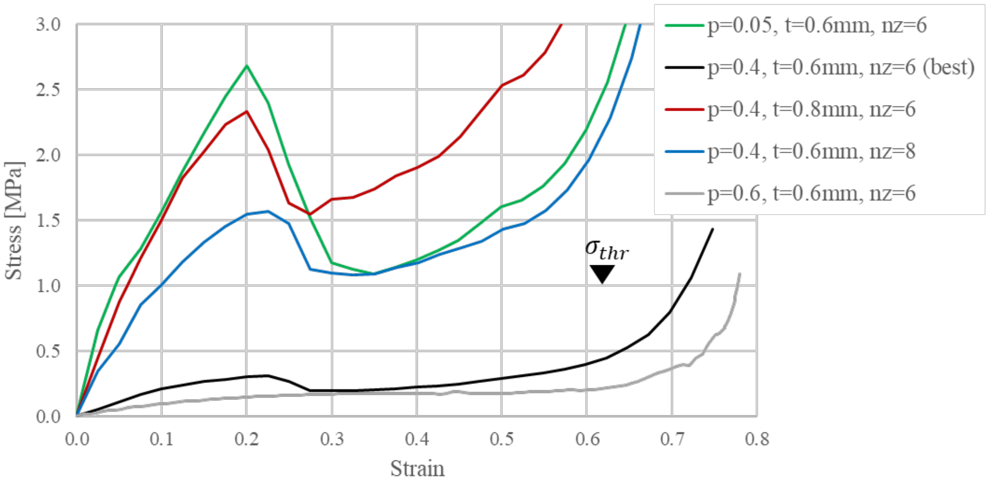

Fig. 7. Stress-strain curves compression for different values of prebuckling (p), wall thickness (t), and folds in the loading direction (nz).

Finally, some of the designs were fabricated and tested for validation purposes. We used the fuse filament fabrication (FFF) method, with Prusament TPU 95A (having Shore A hardness 95) as the base material (filament). Figure 8 shows the stress-strain curve under compression for the best sample ($p = 0.6$, $t = 0.6$ mm, and $n_z = 6$), as determined using Abaqus and experimentally. Beyond the uncertainties in the numerical model (material, boundary conditions, contact properties) to reproduce the experiment, numerical and experimental results show a satisfactory agreement. The absorbed energy is noteworthy well predicted: 0.225 MPa from the Abaqus' results, 0.220 MPa from the experiment.

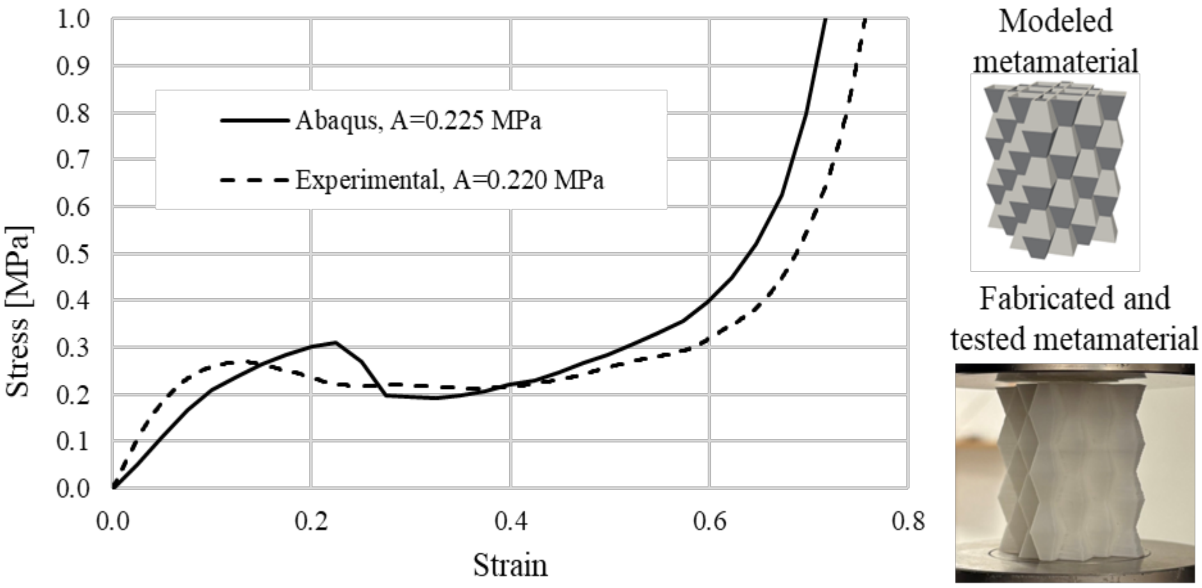

Fig. 8. Experimental and numerical stress-strain curves and absorbed energy per unit volume (A) below 1 MPa stress threshold for the metamaterial on the right.

Conclusion

In this work, we define a unique parameterised metamaterial that unifies recently proposed origami honeycombs [1] and plate-lattice metamaterials [2], both shown to outperform conventional foams in energy absorption and impact mitigation.

An evolutionary optimisation is performed to maximise energy absorption while constraining the peak stress below a prescribed threshold, using the metamaterial parameters as design variables. For each candidate design, the objective function-defined as the absorbed energy per unit volume over the strain interval from zero up to the strain at which the peak stress reaches the threshold—is computed by integrating the stress-strain response obtained from finite element simulations of compression tests. These simulations are conducted using the commercial software Abaqus, selected for the robustness of its general contact formulation. However, the high licensing cost of Abaqus obliged us to adopt an over-constrained design space containing a small number of design variables (pre-buckling, wall thickness, and number of folds), few discrete levels for each, and to allow a low total number of objective function evaluations in the optimization process. That's why we prefer to call "best" instead of "optimal" the design resulting from the current optimization process.

Despite these limitations, the results clarify the central roles of buckling and contact: the former limits the initial stress peak, while the latter enhances post-buckling energy absorption. The findings further indicate substantial potential for achieving truly optimal metamaterial designs by exploiting the full geometric freedom afforded by additive manufacturing to define a richer design space. But this richer design space should be adequately explored, which requires to avoid licensing constraints. So, future work will focus on identifying free software with robust contact algorithms capable of handling large deformations.

Acknowledgment

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