# Supplementary Materials

## Analysis of the role of the penalty factor $p$

A penalty factor of 3 is commonly used in the topology optimization of problems dealing with solid materials, where a discrete "black and white" design is preferred, i.e., the intermediate density is penalized to values either close to 1 or 0 such that the domains of the solid material (density of 1) and the voids (density of 0) can be clearly distinguished. In this work, on the other hand, we seek a continuous transition of the lattice gradient, where intermediate values of density between 0 and 1 are preferred as they represent the homogenized relative density of the corresponding lattice material. For this reason, we decrease the penalty factor from 3 to 1.

Having stated the above rationale, we observe that a penalty factor of 1 can still yield a black-and-white distribution of relative density in a TPMS lattice, such as in our Gyroid in Figure 3(a), reported again below as Figure S1(a). The reason for this can be attributed to the relation between the independent homogenized elastic constants ( $D_{ij}^H$ ) and the relative density of a Gyroid lattice ( $\rho^{(e)}$). This relation is given by:

$$D_{ij}^H = D_{ij}^*(a_{ij}e^{b_{ij}\rho^{(e)}} - a_{ij}), \tag{1}$$

where ( $D_{ij}^*$ ) are the elasticity constants of the solid material, and $a_{ij}$ as well as $b_{ij}$ are constants obtained from numerical homogenization. As can be observed from Eq. (10), the exponential term $e^{b_{ij}\rho^{(e)}}$ is used to fit the material effective properties; its expression resembles the penalty term appearing in the topology optimization formulation. From this resemblance, we can observe that the material model of a TPMS lattice acts as a pseudo-penalty function, which appears before the true penalty term of topology optimization is applied. The tendency to yield a discrete "black-and-white" distribution of density is here exacerbated by the exponential term of the material model.

To demonstrate that the cause for a black-and-white distribution appearing in the Gyroid lattice upon the application of a penalty factor of 1 is due to the exponent of the material fitting (Eq. 10), which resembles the form of the penalty function in the topology optimization formulation, we carry out a controlled numerical experiment. We examine a classical iso-truss lattice[24, 1], and compare it with the Gyroid lattice proposed in this work. For both of them, we apply a penalty factor 1, prescribe identical terms in the topology optimization formulation, and then compare the outcome, i.e., the relative density distribution.

For the iso-truss lattice, we recall the effective material properties fitted through a non-exponential regression model[2] are given by the following higher-order polynomial [24]:

$$\frac{E^H}{E^s} = (0.20529 - 0.03303\nu^s)\rho + (0.08121 + 0.27243\nu^s)\rho^2 + (0.64974 - 0.24237\nu)\rho^3 \tag{1}$$

where $E^H$ is the homogenized Young's modulus, $E^s$ the Young's modulus of the solid material, $\nu^s$ the Poisson's ratio, and $\rho$ the relative density. Figures S1(a) and S1(b) show the results. The former shows that regions with high relative density originate from both the top corners of the support domain, and propagate diagonally towards the centre of the printing base; another dense agglomeration is generated from the cantilever tip vertically to the base. The latter shows a similar trend although the transition between high- and low-density regions is smeared; this leaves a considerably smoother gradient pattern in the iso-truss than in the Gyroid lattice.

From the results above, we can infer that the appearance of a black-and-white distribution of relative density in a Gyroid lattice is mainly governed by the effective properties of the material model (Eq. 10). Therefore we can conclude that if the regression model of the effective material property resembles the exponential term in the penalty function, the yielded design tend to display a sharper transition between regions of high and low density values.

Besides the explanation above, we want to emphasize additional points that pertain to the practical use of truss-based lattices. Although the use of a truss-based lattice can promote gradient smoothness in the numerical solution (Figure S1(b)), the drawbacks can be significant in the context of 3D printing. Truss-based lattices with inclined and inter-connected bars manufactured via LPBF are prone to imperfections[3, 4], making them a less favourable choice compared to shell-based lattices with continuous surfaces. Furthermore, shell-based lattices (e.g., TPMS lattices) feature prominent advantages for LPBF, such as a propensity to lead to a more uniform stress distribution than strut-based lattices, and high surface area-to-volume ratio, a factor yielding a better thermal dissipation capacity than conventional truss-based lattices.

## Topology optimization formulation and additional details

The state function ($K(D^H(\rho_e))U(\rho_e) = F_{\text{inh}}$) in the problem formulation is necessary to calculate the unknown displacement fields $U$, a fundamental dependent variable for the obtainment of the objective and associated gradient (a.k.a sensitivity analysis). $K$ is the global stiffness matrix, which is the assembly of all elementary stiffness matrices of the design element $k^{(e)}$, in this work, an eight-node linear hexahedral element. To derive $k^{(e)}$ for a voxel element, we use the method of the potential energy:

$$k^{(e)} = \int_{\Omega^{(e)}} B^T D^H(\rho^{(e)}) B d\Omega^{(e)}, \tag{3}$$

where $B$ is the strain-displacement matrix of the linear hexahedral element, $D^H(\rho^{(e)})$ is the homogenized elasticity tensor obtained through the method described in Section 2.3, and $\Omega^{(e)}$ is the voxel $e$'s volume. In the state function, $F_{\text{inh}}$ ,is the global force vector, which is the assembly of all elemental strain-induced forces $f_i^{(e)}$, whose derivation is given in Section 2.2. For completeness, we reproduce the equation here:

$$f_i^{(e)} = \int_{\Omega^{(e)}} B_i^{T(e)} D_i^{(e)} \varepsilon^{inh} d\Omega_i^{(e)} \tag{4}$$

We can solve for $U(\rho_e)$ by backward substitution (12), (13) into the state equilibrium function $K(D^H(\rho_e))U(\rho_e) = F_{\text{inh}}$.

The sensitivity analysis can be performed upon obtaining the displacement field $U$. The objective value, i.e., the compliance of the overall cantilever beam, depends on the material properties of each element, which can be fitted as a function of the relative density of each element $\rho_i$. Hence, the partial derivatives of the compliance with respect to the variation of $\rho_i$ can be expressed by substituting the state function into the objective function as:

$$\frac{\partial C}{\partial \rho_i} = F_{\text{inh}}^T \frac{\partial U(\rho_i)}{\partial \rho_i} = U^T(\rho_i)K(\rho)\frac{\partial U(\rho_i)}{\partial \rho_i} \tag{5}$$

Given $F_{\text{inh}}^T$ is an independent inherent force vector, calculating the total derivative of the state equation with respect to $\rho_i$ yields:

$$\frac{\partial K(\rho_i)}{\partial \rho_i}U(\rho_i) + K(\rho_i)\frac{\partial U(\rho_i)}{\partial \rho_i} = 0 \Rightarrow \frac{\partial U(\rho_i)}{\partial \rho_i} = -K^{-1}(\rho_i)\frac{\partial K(\rho_i)}{\partial \rho_i}U(\rho_i) \tag{6}$$

Substituting (15) into (14) yields the final form of the sensitivity of the objective function with respect to the design variable $\rho_i$:

$$\frac{\partial C(\rho_i)}{\partial \rho_i} = -U^T(\rho_i)\frac{\partial K(\rho_i)}{\partial \rho_i}U(\rho_i) \tag{7}$$

The stiffness of the solid material $k_0^{(e)}$ in the modified SIMP method [56] is thus penalized by a factor of $p$ that is governed by the element density $\rho_i$:

$$k^{(e)}(\rho_i) = [E_{\min} + \rho_i^p(E_0 - E_{\min})]k_0^{(e)}, \tag{8}$$

where the penalized stiffness $k^{(e)}(\rho_i)$ in (17) is substituted in (16) to obtain the final form of the objective sensitivity (Eq. 6)

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Figure S1: Comparison of optimized gradient of volume fraction (relative density) obtained with a penalty factor of 1 for (a) Gyroid lattice and (b) iso-truss lattice