Imperfections: using defects to program designer matter

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Title: Imperfections: using defects to program designer matter
Issue Date: 2021-05-26

2. A spin-ice-inspired class of complex metamaterials[1]

Abstract

The basic tenet of metamaterials is that architecture controls the physics[7–10,15–22]. So far, mainly defect-free architectures have been considered. However, defects, and particularly topological defects, play a crucial role in natural materials[23–27]. Here we provide a systematic strategy to introduce such defects in mechanical metamaterials. We first present metamaterials that are a mechanical analogue of spin systems with tunable ferromagnetic and antiferromagnetic interactions; then design an exponential number of frustration-free metamaterials; show how we can introduce local defects by rotating specific building blocks; and finally introduce topological defects by rotating a string of building blocks in these metamaterials. Our work presents a new avenue to systematically include spatial complexity, frustration, and topology in mechanical metamaterials.

2.1. Introduction

Mechanical metamaterials are structured forms of matter with unprecedented properties, including negative response parameters[15], shape-morphing[7,8], topological mechanics[16–19], and self-folding[9]. While the focus has been on frustration-free compatible architectures, where all unit cells deform in harmony, frustration causes more complex, higher-energy deformations, leading to advanced functionalities, such as multistability and programmability[10,20–22], and may open up opportunities to probe controlled frustration in man-made systems[23–25]. We note that deformations of unit cells in compatible metamaterials often alternate, leading to horizontal and vertical ellipses[15], rigid elements that rotate left or right[10,28,29], or edges of unit cells that move in or out[7,22]: we refer to this as *antiferromagnetic order*. Hence, a promising route to introduce targeted frustration is to use fundamental building blocks that favour either antiferromagnetic order or ferromagnetic, non-alternating order, and use the freedom supplied by additive manufacturing to stack these at will. Paths connecting pairs of such building blocks carry a *parity*, given by the parity of the number of antiferromagnetic interactions along the path. In compatible architectures, all paths connecting any pair of building blocks must have the same parity, and we anticipate that we can solve the combinatorial constraints that govern such designs[7,30]. In contrast, generic configurations tend to violate such constraints, leading to frustration and defects.

We start our investigation in section 2.2 by describing simple, 2D triangular building blocks that can be stacked together to interact either ferro- or antiferromagnetically, and that form the basis of our mechanical networks. In section 2.3, we discuss a technique[30] to stack these building blocks into compatible, frustration-free architectures with controllable isotropy and periodicity. A simple design rule to ensure compatibility is formulated,

[1] The work presented in this chapter is based on Refs.[13] and [14].

based on a mapping between the mechanical network and an antiferromagnetic Ising spin-ice. As we show in section 2.4, this simple design rule naturally suggests a protocol to violate compatibility by creating controlled local and topological defects in the network. Finally, we present an outlook and suggestions for further research in section 2.5.

2.2. Triangular building blocks

To implement our design strategy, we now introduce anisotropic, triangular building blocks that set the ferromagnetic or antiferromagnetic nature of their interactions depending on their mutual orientations.

We work with a specific type of mechanical elements consisting of freely hinging nodes connected by bonds modelled as rigid bars. Compatibility in such networks means that there is a single, global mode of motion, called a *floppy motion*, such that the network deforms at zero energy cost- that is, none of the rigid bars change their length during this deformation. In a compatible network consisting of smaller building blocks, it is necessary that each of the individual building blocks is compatible as well, and has what we call a *local floppy mode*.

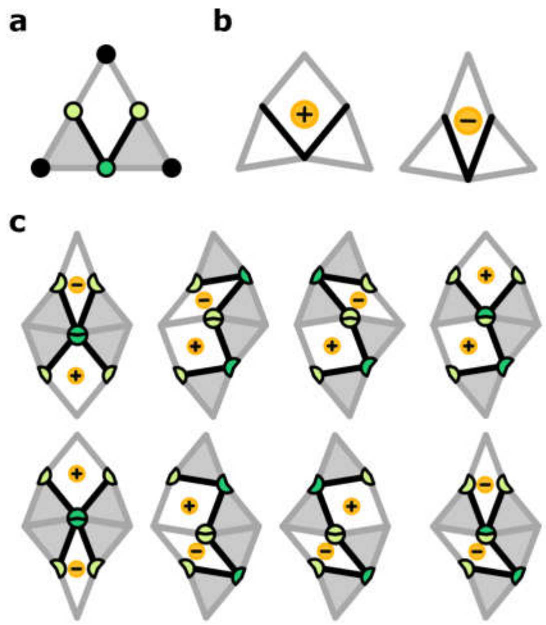

Fig. 2.1.: Stackable building block. a, Anisotropic building blocks consisting of edge bonds (grey), internal bonds (black), corner nodes (black), majority edge-nodes (light green), and a minority edge-node (dark green). **b**, Deformed building block in fat (+) and skinny (-) states. **c**, Adjacent building blocks may be stacked together in four distinct configurations (columns). Each configuration can be deformed in two ways (top and bottom rows). Adjacent building blocks interact antiferromagnetically (ferromagnetically) when their shared edge features an even (odd) number of minority nodes, so that their minority nodes are connected by an even (odd) number of internal bonds.

We use the triangular building block shown in Fig. 2.1a. Each block consists of six nodes in a triangle configuration in the (x, y)-plane. The six nodes are positioned at integer multiples of two triangular basis vectors $\boldsymbol{a}_1 = l(1, 0)$ and $\boldsymbol{a}_2 = l(1/2, \sqrt{3}/2)$, where the lattice parameter l may be chosen freely. We distinguish three *corner nodes* at the triangle's corners, and three *edge nodes* (of which two are *majority edge-nodes* and one a *minority edge-node*) halfway the triangle's edges. The nodes are connected by eight bonds: six *edge bonds* around the triangle's perimeter, and two *internal bonds* connecting the majority nodes to the minority node, so that all bonds have length l. This leaves the two minority nodes unconnected to each other, and results in an anisotropic building block.

The triangular building block features a floppy "hinging" motion, illustrated in Fig. 2.1b (see Appendix A.1 for details), which allows the block to deform at zero energy cost as

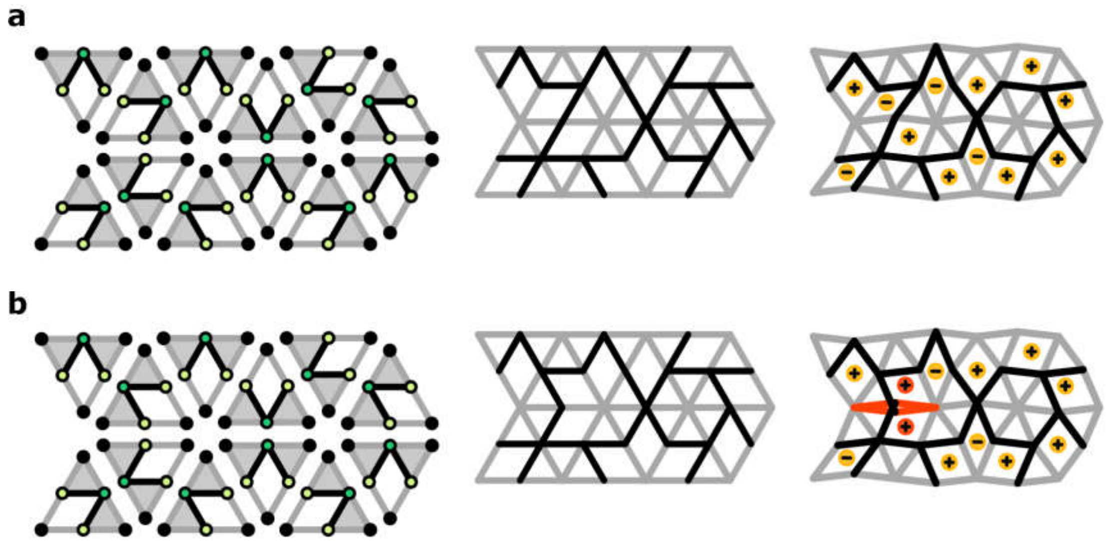

Fig. 2.2.: Randomly stacking building blocks produces floppy or frustrated networks. **a**, Stacking building blocks with various orientations on a triangular lattice (left) produces a metamaterial consisting of rigid bars connected by freely hinging joints (middle). The particular example shown exhibits a floppy mode: the blocks undergo a collective deformation and fit together like puzzle pieces (right). **b**, A slightly different random stacking is frustrated, as indicated by the red block spins and edge bonds: there is no collective deformation of the building blocks so that all deformed blocks fit together.

all bond lengths remain constant. Accordingly deformed building blocks can take on two shapes—fat and skinny—which we assign a positive or negative *block spin* variable.

When two building blocks are stacked together, they exhibit a collective floppy deformation: the two blocks deform together, each becoming either fat (positive block spin) or skinny (negative block spin). There are four unique ways to stack a block pair (Fig. 2.1c), and the relative floppy deformation of the two blocks depends on how they are stacked together. When their shared edge contains one minority node, the building blocks interact *ferromagnetically*: the zero-energy deformation then features two building blocks with the same block spin. In contrast, when their shared edge possesses either zero or two minority nodes, the interaction is said to be *antiferromagnetic*, and the deformations have opposite block spins.

2.3. Compatible metamaterials

To create metamaterials consisting of many building blocks, we stack blocks on a triangular lattice with varying orientations (Fig. 2.2). This stacking method allows us to design structures with a wide range of structurally complex geometries. Such stacked metamaterials can be either compatible, so that the stack can deform at zero energy cost (Fig. 2.2a), or frustrated (Fig. 2.2b). Stacks with randomly oriented building blocks are usually frustrated. To obtain *targeted* frustration, we start in this section by first designing compatible, frustration-free configurations, before introducing controlled frustration. That is, we formulate design rules for metamaterials where all building blocks deform simultaneously according to their local floppy mode, so that the deformed building blocks fit as in a jigsaw puzzle.

In section 2.3.1, we first show that frustration-free configurations require that in each hexagon of six adjacent building blocks, the number of connected antiferromagnetic interactions, corresponding to the smallest possible closed *local loop* of internal bonds, is even. This finding implies that compatibility is equivalent to requiring that all local loops are of even length (Fig. 1d,e; see methods) while odd local loops generate frustration[31].

A vast number of structurally complex configurations satisfy the above compatibility condition. Counting and designing these geometries requires solving combinatorial problems. In section section 2.3.2), we explore their solutions. Since all compatible architectures feature a floppy mode where all building blocks have two edge nodes moving "in" and one minority edge-node moving "out" (or vice versa), we can map these deformations to ground states of an antiferromagnetic Ising model on the kagome lattice (*AFIK model*). Each ground state of this AFIK model generates a distinct compatible metamaterial, up to a global spin flip. The extensive ground-state entropy of that model[32,33] yields an asymptotically exact result for the exponential number of compatible architectures as a function of the system size[30]. We show in section 2.3.3 that this rich design space allows us to create structures with a wide range of secondary properties, such as (an)isotropy and periodicity.

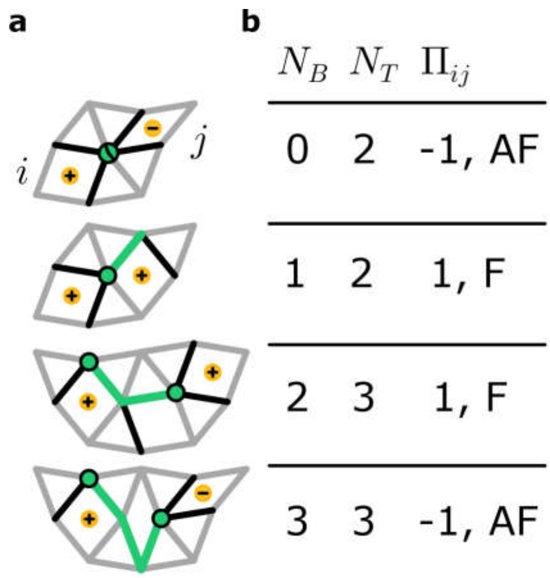

Fig. 2.3.: Path parity. a, Four stacks where pairs i, j of building blocks are interconnected. When blocks i, j undergo a floppy deformation, they either extend (+) or contract (-). **b**, The relative sign of the blocks' deformations depends on the length N_B of the connecting path of internal bonds (green lines), which runs from the minority node of block i to that of block j (green circles), and the number of connecting blocks N_T. A path parity $\Pi = (-1)^{N_b - N_T - 1}$ may be defined so that the block deformations of i and j are identical (different) if $\Pi = 1$ ($\Pi = -1$), corresponding to a ferromagnetic, 'F' (antiferromagnetic, 'AF') interaction between i and j.

Finally, in section 2.3.4, we discuss an important example of a frustration-free geometry: an ordered metamaterial where all interactions between block spins are antiferromagnetic. Its zero-energy deformation mode has all up-facing (down-facing) building blocks in their fat (skinny) state, or vice-versa, which corresponds to alternating positive and negative block spins. We note that this geometry is equivalent to the rotating square mechanism that underlies the design of a wide range of metamaterials[9,15,20,28,29,34]. More generally, geometries with fully antiferromagnetic block spins can be mapped to diamond tilings, where each diamond represents two building blocks with two minority nodes on their shared edge. We show that the number of possible fully antiferromagnetic designs grows exponentially with system size.

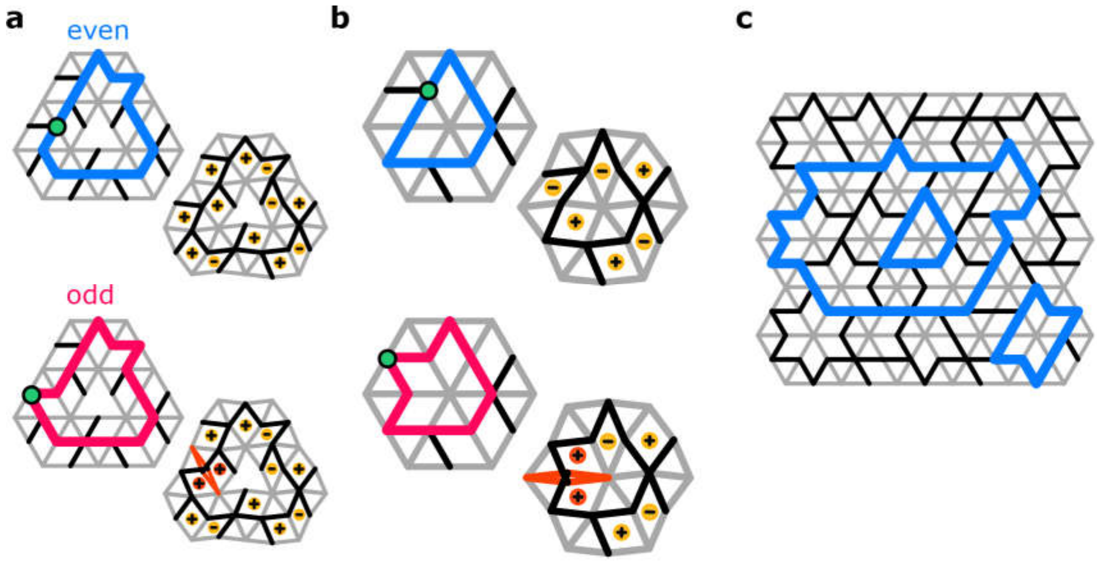

Fig. 2.4.: Compatible structures satisfy a parity rule for closed paths. **a**, A building block (minority node highlighted in dark green) is connected to itself on a triangular lattice via an even number of neighbours. Top: a loop of an even number of internal bonds (bold blue lines) runs around the cluster, ensuring that the building block interacts ferromagnetically with itself. The cluster has a floppy mode. Bottom: an odd loop (bold red lines) produces an antiferromagnetic self-interaction and leads to frustration (red edge bonds). There is no floppy mode. **b**, *Local loops* within a superhexagon of six blocks form the smallest possible closed paths of internal bonds. An even (odd) local loop produces a compatible (incompatible) hexagonal structure. **c**, If all local loops in a metamaterial are even, all larger loops are, too. Thus, evenness of each local loop ensures compatibility.

2.3.1. Parity of paths of internal bonds

As discussed above, in a compatible metamaterial, all building blocks can simultaneously deform according to their local floppy mode. We conceive of the joint floppy deformation of any pair i, j of blocks, connected by a larger cluster of building blocks, as an interaction. Examples are shown in Fig. 2.3a. For a *ferromagnetic* interaction, the blocks have the same block spin and simultaneously expand or simultaneously contract, whereas for an *antiferromagnetic* interaction the blocks' spins are opposite: one block contracts while the other expands. We show here that the internal bonds connecting blocks i, j determine their interaction type, and we formulate a design rule for the internal bonds to ensure that all blocks in a metamaterial can deform simultaneously.

We define a *path* of N_b internal bonds running from the minority node of block i to the minority node of block j through their connecting cluster of building blocks, and define N_T as the number of triangular building blocks traversed by the path (including blocks i and j). The *path parity*

$$\Pi = (-1)^{N_b - N_T - 1} \tag{2.1}$$

is then positive (negative) when the interaction between i and j is ferromagnetic (antiferromagnetic), as illustrated in Fig. 2.3b.

This path parity rule leads to a self-consistency requirement for closed paths, or *loops* of internal bonds, running from any block i to itself. After all, the block must interact

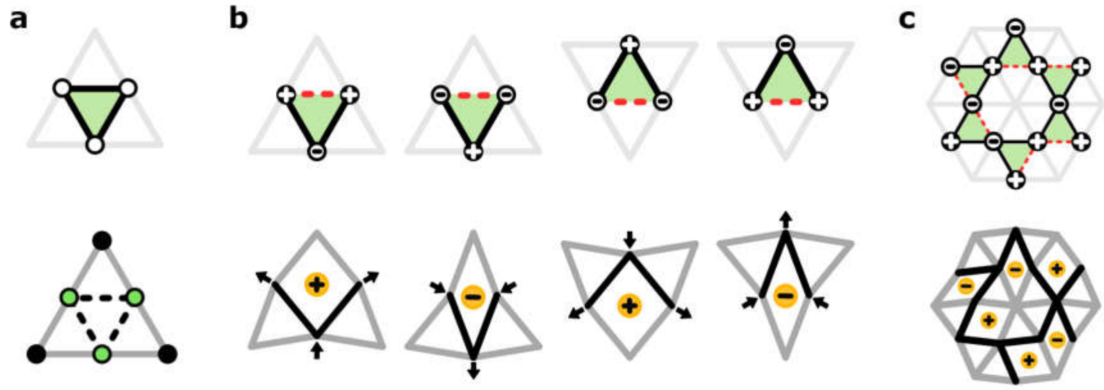

Fig. 2.5.: Compatible structures can be designed with a spin mapping. **a**, Top: a unit cell (light grey outline) of an Ising model on a kagome lattice (green triangle). Edge spin sites (open circles) are connected by antiferromagnetic interactions (black bars). Bottom: the spin cell maps to a mechanical building block with three corner nodes (black circles), six edge bonds (dark grey bars), and three possible internal bonds (dashed black lines) that connect the three edge nodes (green circles). **b**, Ground states of the spin cell (top) map to a mechanical building block with a prescribed floppy mode (bottom). Satisfied antiferromagnetic interactions correspond to internal bonds; the unsatisfied spin interaction (red dashed line) signifies an absence of bonds. Positive (negative) edge spins map to outward (inward) edge node deflections of the upward- (downward-)pointing mechanical blocks. **c**, Top: a spin ground state of a hexagonal section of the kagome lattice. Bottom: corresponding hexagonal mechanical metamaterial, which possesses a floppy mode obtained directly from the spin ground state.

ferromagnetically with itself in order to deform compatibly. Equivalently, the path parity of a loop containing the block must be positive. We can re-formulate this path parity condition, using the fact that any closed path on a triangular lattice traverses an even number of triangles. Hence, to ensure that a building block interacts ferromagnetically with itself, we must ensure that the parity of the number of internal bonds in the loop must be even; equivalently, that the number of minority nodes on shared edges is even; and that the number of (anti)ferromagnetic interactions between adjacent blocks in the path is even.

In a compatible network, all closed paths must therefore contain an even number of internal bonds. Conversely, loops with an odd number of internal bonds imply incompatibility. Fig. 2.4a shows an example of a compatible closed path with even length, and a frustrated closed path with odd length. Due to the structure of our building blocks, each lattice point—where the blocks' corner nodes meet—is circumscribed by a *local loop* within a hexagon of six adjacent blocks, which we will refer to as a *superhexagon*; two examples are shown in Fig. 2.4b. Such local loops are the smallest closed paths of internal bonds in our networks, and must all satisfy the self-consistency requirement to ensure compatibility. Conveniently, when all local loops in a metamaterial satisfy the compatibility requirement, larger loops are guaranteed to contain an even number of internal bonds as well (Fig. 2.4c). In summary, if and only if a network is compatible, then all loops of internal bonds—-from the smallest local loops around each lattice point to the largest loops around the network boundary—have an even number of bonds in their perimeter.

2.3.2. Mapping compatible metamaterials to an antiferromagnetic Ising model on the kagome lattice

The above parity rule helps us identify which structures are compatible. However, this parity rule does not help us design compatible structures from scratch. We address this issue here.

To obtain a design strategy for compatible metamaterials, we map the local FM of a building block to the ground state of an Ising spin model with antiferromagnetic interactions on the kagome lattice (AFIK model)[13] as illustrated in Fig. 2.5a. We associate a positive (negative) binary edge spin variable to an extensile (contractile) edge node deflection for a downward-pointing building block, and vice versa for upward-pointing blocks (Fig. 2.5b). In the AFIK model, the three spin sites inside a building block are connected by three antiferromagnetic interactions. These three interactions cannot be simultaneously satisfied: the lowest-energy spin configuration satisfies only two of the antiferromagnetic interactions, and violates one. The building block's mechanical FM corresponds to such a minimal-energy spin configuration that satisfies two out of the three antiferromagnetic interactions. Specifically, the building block's two internal bonds connect edge spin sites in opposite states, while the edge nodes not connected by an internal bond both move inward (or both outward), representing a frustrated antiferromagnetic interaction. Hence, the lowest-energy AFIK configuration corresponds to the local floppy mode of a single building block.

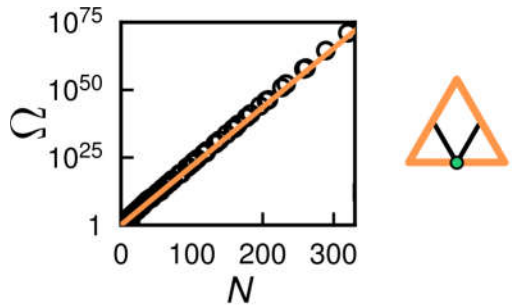

Fig. 2.6.: Counting compatible designs. The numerically obtained number of compatible designs Ω is shown as a function of the number of edge nodes N and compared to asymptotic predictions based on an Ising-spin mapping. An exact count of the number of compatible parallellogram-shaped designs[30](circles), created by combining building blocks (top right, orange triangle) in various orientations, closely matches the ground-state degeneracy of the corresponding Ising model (orange line)[32].

Adjacent blocks deform compatibly when their shared edge spins match. Thus, in compatible architectures, the edge spins form a kagome lattice where each triangular plaquette features one positive and two negative edge spins, or vice versa (Fig. 2.5c). Such collective edge spin states are precisely the degenerate ground states of the AFIK model, so that each ground-state configuration generates a distinct compatible metamaterial (up to a global spin flip).

We note here that this mapping to an Ising model with binary states is complete only for compatible metamaterials which possess a FM in which displacements alternate in direction and all have the same magnitude. As we show in the following chapter, in incompatible structures, the magnitude of the displacements varies continuously with position. In that case, the mapping to the Ising model serves only to demonstrate whether there exists a global compatible deformation.

From the AFIK mapping, we obtain an asymptotic expression for Ω_0, the number of compatible architectures, via the residual entropy $S_0 \approx 0.502N$ of the degenerate ground state of the AFIK model[32,33]

$$\Omega_0 \sim e^{0.502N} = e^{0.753T} \approx 2.1^T < 3^T = \Omega_{tot}, \tag{2.2}$$

where N denotes the number of edge spins, T the number of blocks, $N = 3T/2$ the number of edge spins in the thermodynamic limit, and Ω_{tot} the total number of architectures. The asymptotic expression agrees well with the exact number of compatible, parallelogram-shaped architectures as determined by computer algorithms[30], even for small systems (Fig. 2.6).

2.3.3. Diversity of compatible metamaterial architectures

With the AFIK mapping described above, we find that an exponential number of compatible designs can be constructed as a function of the design's size. While this implies that we can find compatible architectures with a wide range of secondary properties that arise from symmetries (such as isotropy and periodicity), the structures do share a special feature: their total area decreases under actuation of their floppy mode. Here, we discuss these two design aspects—symmetry and shrinking—briefly.

First, stacking building blocks with varying degrees of disorder produces metamaterials with more or less symmetry. Two order parameters that help describe symmetries are isotropy and periodicity. Isotropic materials are rotationally symmetric, and have the same properties in all radial directions. Conversely, periodic structures have translational symmetries, and are invariant under some discrete translations. While a prescriptive approach to constructing metamaterials with specific symmetries is outside the scope of this work, the framework used here, where we treat metamaterials as stacks of simple building blocks, invites intuitive design. That is, structures with more or less order can be found by stacking and rotating the building blocks heuristically. Some products of this approach are shown in Fig. 2.7, where four structures of varying (an)isotropy and (a)periodicity are shown.

Secondly, during floppy deformation of any compatible stack, about half of the building blocks will expand, while the other half contracts. Contraction of a building block produces a larger area change than extension, as we show below, and as a result, the total area of the metamaterial tends to decrease.

We can understand this shrinking behaviour using our knowledge of the net ground state magnetization of the AFIK model[35], and the geometry of the building blocks during deformation. We use the fact that a compatible stack of building blocks can also be seen as a stack of even local loops on a triangular mesh background, as discussed in section 2.3.1. We illustrate this concept in Fig. 2.8: Fig. 2.8a shows the eight possible shapes that even local loops inside a superhexagon of six adjacent building blocks can take, barring rotations and reflections. The local loop determines whether some of the building blocks it traverses expand or contract, as illustrated in Fig. 2.8b. Specifically, when a building block's deforming quadrangle lies inside the local loop, its deformation with respect to its loop-mates is fixed. In this way, the shape of the local loop sets the deformation of 0, 2, 4, or 6 building blocks. Inspection shows that each even local loop enforces an equal

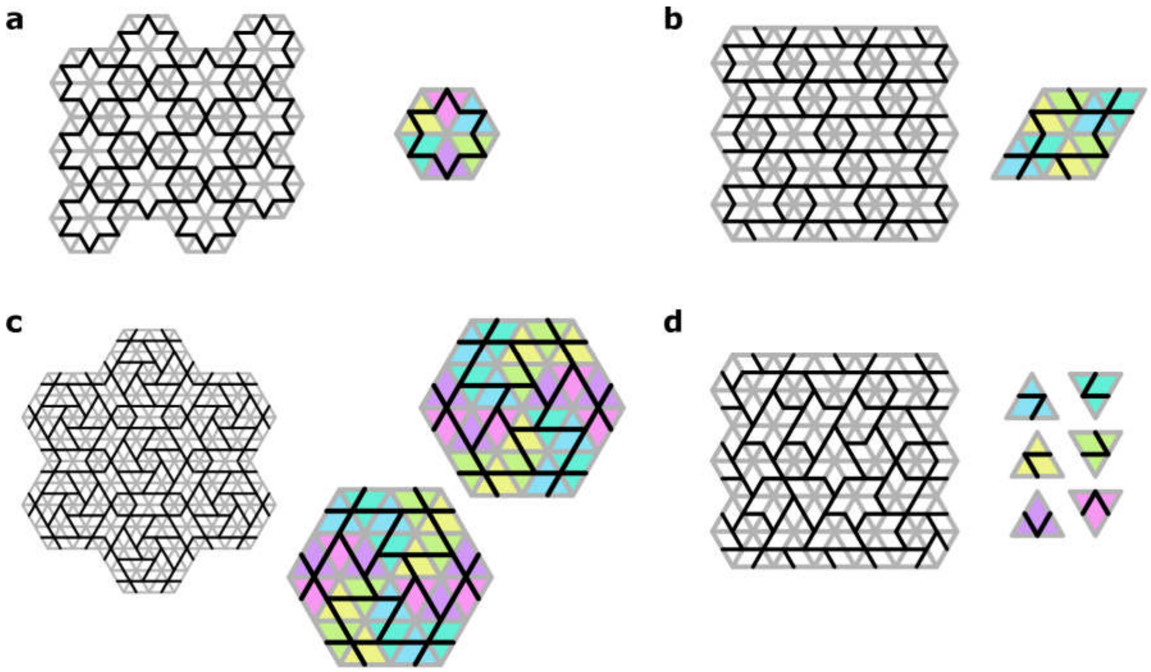

Fig. 2.7.: Compatible designs come in a wide array of (dis)order. **a**, An isotropic and periodic design (left) is highly ordered. Isotropic unit cells (right), which feature an equal number of building blocks in each of the six possible orientations (colours), create this architecture. **b**, An anisotropic yet periodic design (left) is created by stacking anisotropic unit cells (right), which contain an unequal number of building blocks in the six block orientations. **c**, An isotropic and aperiodic design (left) is made by stacking together isotropic unit cells (right). Periodicity is avoided here by stacking mirrored copies of the unit cells in a random arrangement. **d**, A disordered design (left) which is anisotropic and aperiodic. It is constructed by randomly stacking building blocks in different orientations, while respecting compatibility (right).

number of expanding and contracting building blocks. Thus, the number of expanding and contracting building blocks in a stack of even loops is equal. In a corresponding stack of triangular building blocks, this equality can only be violated at the system's boundary: there is a local design freedom to introduce more expanding or more contracting building blocks at the material's edges. An example is shown in Fig. 2.8c. In the limit of large system sizes however, the boundary contributes an eventually vanishing fraction to the total number of building blocks. As a result, half of the blocks contract and half expand during an infinitely large compatible stack's floppy deformation.

As a corollary, the area of a compatible stack decreases on average during deformation away from its initial shape. This follows from some trigonometry. Consider a building block with an opening angle $\theta_0 + \Delta\theta$ between its two internal bonds, where θ_0 is the rest opening angle and $\Delta\theta$ the deviation from the resting value during its floppy deformation (Fig. 2.9a). The area A spanned by the building block's quadrangle—the only portion that changes shape—is then given by

$$A = l^2 \sin(\theta_0 + \Delta\theta) \ , \tag{2.3}$$

where l is the bond length (Fig. 2.9b). During deformation of a compatible stack, $|\Delta\theta|$ is the deformation's control parameter: it is equal for all building blocks due to geometric

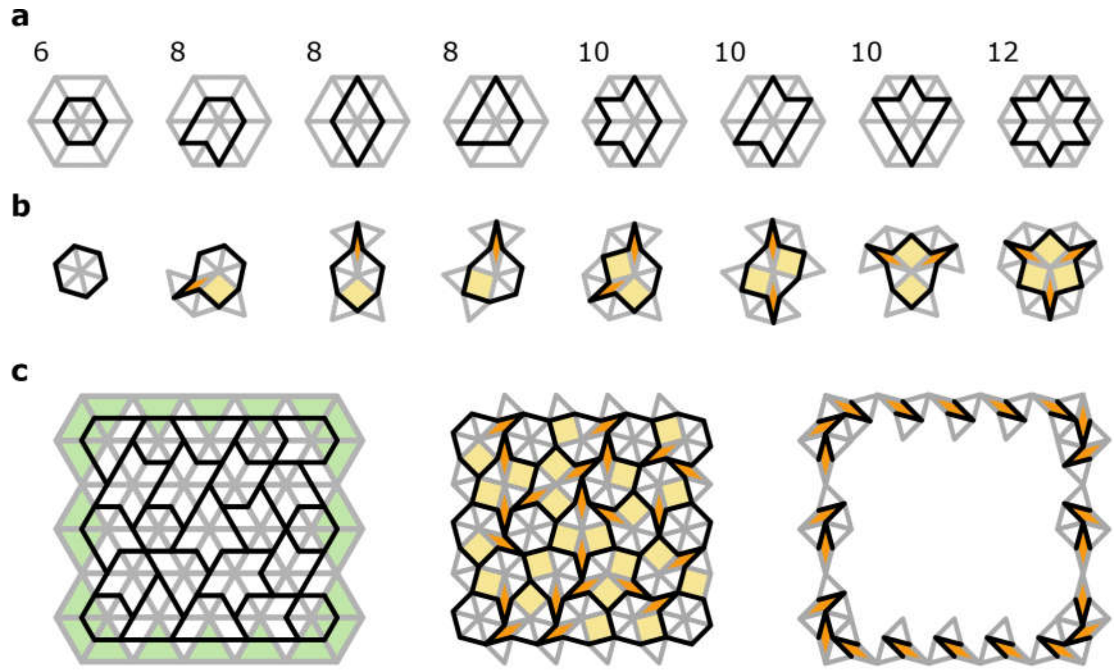

Fig. 2.8.: Compatible designs feature an approximately equal number of contracting and extending building blocks. **a**, The bulk of a compatible architecture can be created by stacking together even local loops (black bars), each contained in a hexagonal backing structure (grey bars). The eight unique even local loops are pictured and the number of internal bonds indicated. **b**, The shape of the local loop governs its deformation as shown. Each local loop sets the extension (yellow) and contraction (orange) of an equal number of triangular building blocks: 0, 1, 2, or 3. **c**, Compatible stacks can be given an unequal number of contracting and extending building blocks by exploiting the boundary. Left: an example is shown of a compatible bulk structure consisting of stacked even loops, with an open boundary (green). Middle: the structure's bulk deformation is fully determined. Right: the edge is freely decorated with arbitrary numbers of extending and contracting building blocks. Here, all boundary blocks contract.

constraints (Fig. 2.9c). Therefore, half of the building blocks increase in area, and half decrease. The area per building block, averaged over the entire stack, is then found to be

$$\langle A \rangle = l^2 \sin(\theta_0) \cos(\Delta\theta). \tag{2.4}$$

Evidently, the average area is maximal in the initial state, when all building blocks have the same shape (Fig. 2.9d). Deforming the material always decreases its area.

As a consequence, to create structures whose floppy deformation produces a net area increase, a different building block is needed. Such a building block should allow for the construction of stacks in which large clusters of neighbours can interact ferromagnetically. The construction of these specialized building blocks is outside the scope of this work. However, with our existing triangular blocks, it is possible to design compatible stacks with locally ordered patterns of expanding and contracting blocks. We discuss an important example in the following section.

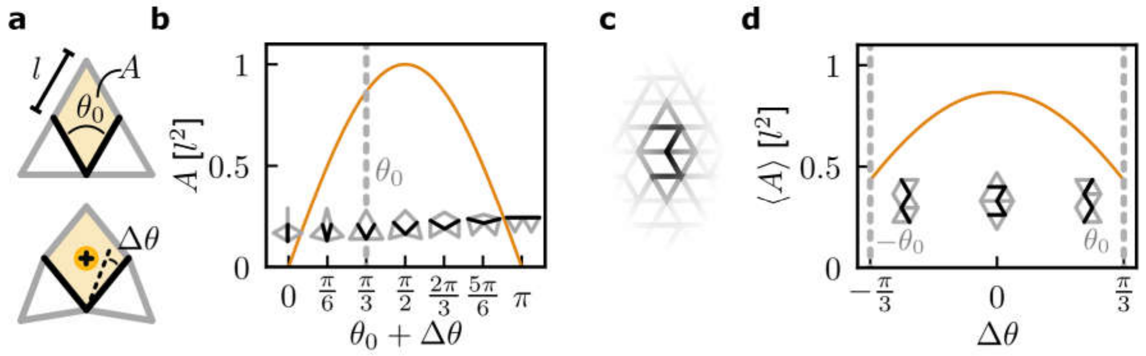

Fig. 2.9.: The area of a compatible architectures decreases under deformation. **a** A single building block with bond length l has a deforming quadrangle of area A (yellow). The deformed shape is set by the rest angle θ_0 between the internal bonds (black bars) and its deviation $\Delta\theta$. **b** Area of the deforming quadrangle as a function of $\theta_0 + \Delta\theta$. Insets show the deformed block shape at indicated angles. **c** In an infinitely large stack, an equal number of building blocks contract and extend. Two antiferromagnetically interacting blocks are shown as an example. **d** The complete stack's average area per block during deformation is shown as a function of angular deviation. The average area per block always decreases away from the rest state at $\Delta\theta = 0$.

2.3.4. Compatible metamaterials with fully antiferromagnetic block spin interactions

Our metamaterial design strategy generates many different network architectures, including the widely-studied rotating square mechanism[9,15,20,28,29,34] illustrated in Fig. 2.10a-b. This is an example of an antiferromagnetic architecture, where all neighbouring building block spins interact antiferromagnetically. Here, we map the design of general antiferromagnetic architectures to the tiling of diamonds and count the resulting number of compatible antiferromagnetic stacks.

Since only building blocks that share zero or two minority nodes interact antiferromagnetically, each building block needs to be oriented so that its minority node is paired with the minority node of one of its neighbours. Identifying such pairs of building blocks as a diamond-shaped tile (Fig. 2.10c), each antiferromagnetic architecture maps to a unique tiling of diamonds. Counting the number of antiferromagnetic architectures thus corresponds to counting diamond tilings, a partition problem of considerable interest in statistical and condensed matter physics[36].

Solutions to this problem yield the number of antiferromagnetic architectures, Ω_{AF}, as a function of the number of edge nodes N. The number of *hexagonal* diamond tilings Ω_{AF} with n diamonds along each hexagon side (e.g. Fig. 2.10c for $n = 2$) can be calculated exactly[37] to be

$$\Omega_{AF} = 2\prod_{i=1}^{n}\prod_{j=1}^{n}\prod_{k=1}^{n}\frac{i+j+k-1}{i+j+k-2}, \tag{2.5}$$

which approaches an exponential function in the thermodynamic limit[38] (Fig. 2.10d):

$$\Omega_{AF} \sim e^{\log(3^{1/2}/2^{2/3})N} \approx e^{0.087N} = e^{0.131T} \approx 1.1^{T}\ , \tag{2.6}$$

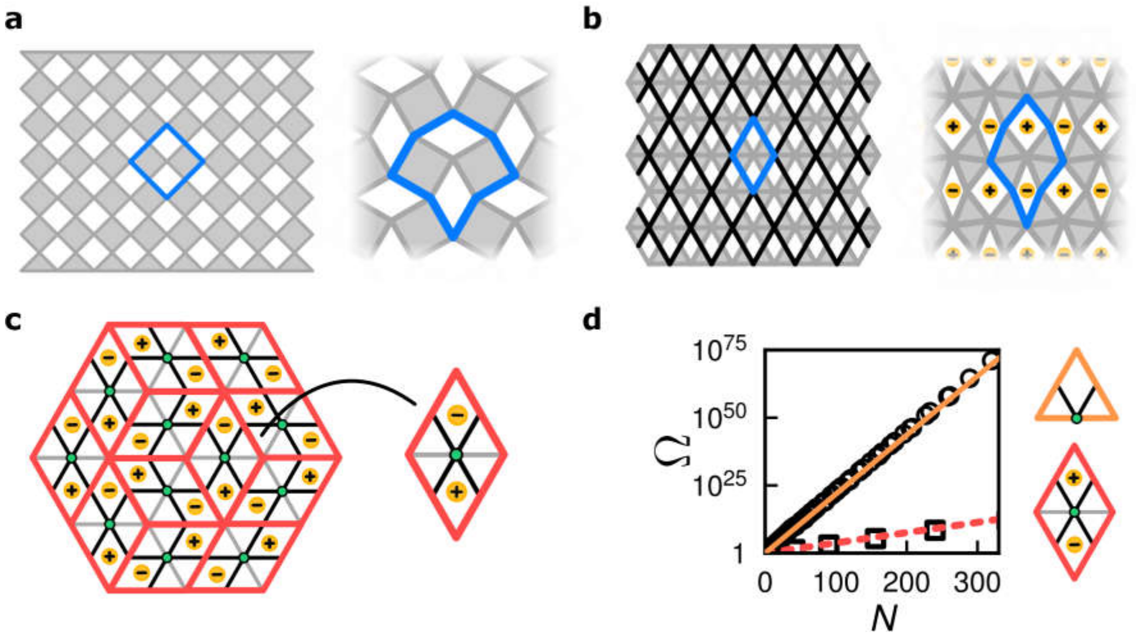

Fig. 2.10.: Counting antiferromagnetic compatible architectures. **a** The rotating square mechanism of rigid squares connected by freely pivoting hinges at rest (left) and deformed (right). The unit cell is highlighted (blue). **a**, Left: the rotating square mechanism is emulated by an ordered compatible stack. Rigid squares are marked in grey. Right: the deformed structure (internal bonds not highlighted). Each building block interacts antiferromagnetically with its neighbours: they have opposite block spin (yellow markers). **c**, All antiferromagnetic designs can be regarded as tilings of diamond-shaped elements (right, red outline) containing two building blocks. The block's minority nodes (green) sit on their shared edge. The blocks deform antiferromagnetically and have opposite block spin. Tiling these diamonds produces hexagonal antiferromagnetic compatible stacks (left). **d**, The number of antiferromagnetic designs Ω (open squares, red dashed line) corresponds to the number of ways diamonds tile a hexagon. It can be counted exactly in the limit of large systems with many edge nodes N (Eq. 2.6). For comparison, the total number of compatible designs (open circles, orange line) is shown.

where $N = 3n(3n + 1)$ is the number of edge nodes, and T is the number of building blocks such that $N = 3T/2$ in the thermodynamic limit.

We now compare the number of antiferromagnetic compatible designs Ω_{AF} to the total number of compatible designs, Ω_0. While Ω_{AF} counts hexagonal systems and Ω_0 parallelogram systems, we expect boundary effects due to the material's shape to be negligible in the limit of large system sizes. We may therefore compare the two cardinalities directly at large N. From Eqs. 2.2 and 2.6, we find that $\Omega_0 \ll \Omega_{AF}$, so that in the thermodynamic limit a vanishing fraction of all compatible architectures has a purely antiferromagnetic interaction pattern (Fig. 2.10d).

2.4. Incompatible metamaterials

As compatible networks require that all local loops of internal bonds are of even length (Fig. 2.4b, top), frustration can be induced by violating this condition. Simply put, we may introduce local loops with an odd number of internal bonds, or *odd local loops* to design targeted frustration (Fig. 2.4b, bottom). Thus, while we can make a large variety of compatible metamaterials, an even larger amount of frustrated designs exist that cannot deform harmoniously due to the presence of one or more odd local loops. The mechanical frustration induced by such defects generally produces undesired effects when their presence is not controlled, such as decay of a desired FM[29,39], or structural failure when frustration-induced bond stresses exceed the bond buckling threshold[40]. However, when frustration is introduced in a controlled and well-understood manner, it may be harnessed to design desirable or unusual physical properties, such as localized buckling zones[13,18,22], or geometric frustration in spin-ices[41–43]. In this section, we show how to introduce frustration in a targeted manner by discrete rotations of the building blocks, which changes the parity of local loops (section 2.4.1). We demonstrate that we can introduce two particular types of frustration, in the form of local, *structural* defects (section 2.4.2) and as global, *topological* defects (section 2.4.3).

2.4.1. Triangle rotations as fundamental architectural transformations

Different architectures are made by stacking together building blocks with different orientations. Therefore, a particular metamaterial design can be transformed into any other architecture by rotating a suitable sequence of building blocks. Supertriangle rotations, illustrated in Fig. 2.11, thus form the minimal architectural transformations that we employ to convert one metamaterial design to another.

Selecting and rotating a particular building block in the material's bulk affects local path parities. Effectively, the rotation removes one of the building block's internal bonds—bond r—from the network and replaces it with a newly added internal bond p (Fig. 2.11a). The bond r is part of up to two local loops: two in the bulk, and one or zero at the material's boundary, as shown in Fig. 2.11b-c. Therefore, exchanging bond r for bond p changes the parity of at most two local loops. This transformation method thus changes local bond connectivity, but preserves other network characteristics, such as the number of nodes and bonds, the node positions, and the bond constraint type.

Starting from a compatible structure containing only even local loops, we can thus obtain metamaterial architectures with isolated, frustrated odd local loops via a suitable sequence of building block rotations. We show below how to implement this strategy to obtain local, *structural* defects, as well as global *topological* defects.

2.4.2. A structural defect

We now show how to locally control frustration in our mechanical metamaterials by rotating a single building block in an initially compatible network.

Fig. 2.12a shows a compatible structure with no defects, where all superhexagons have even local loops (black lines). As discussed in section 2.3.1, all larger paths in a compatible structure enclosing multiple local loops are also even (Fig. 2.4c).

As discussed above, rotating a single building block effectively switches the position of one internal bond, changing the parity of two adjacent even local loops to create two adjacent odd local loops (Fig. 2b), as illustrated in Fig. 2.12a-b. All larger loops circumscribing the two odd local loops are unchanged and are thus still of even length. While the odd local loops frustrate the metamaterial's floppy mode, larger loops around the network perimeter are still even, indicating only a local breakdown of compatibility.

We therefore call two adjacent odd local loops a *structural defect*: while the odd local loops frustrate the material's floppy mode, the defect can be removed by a single local transformation of the network- that is, rotating the block back.

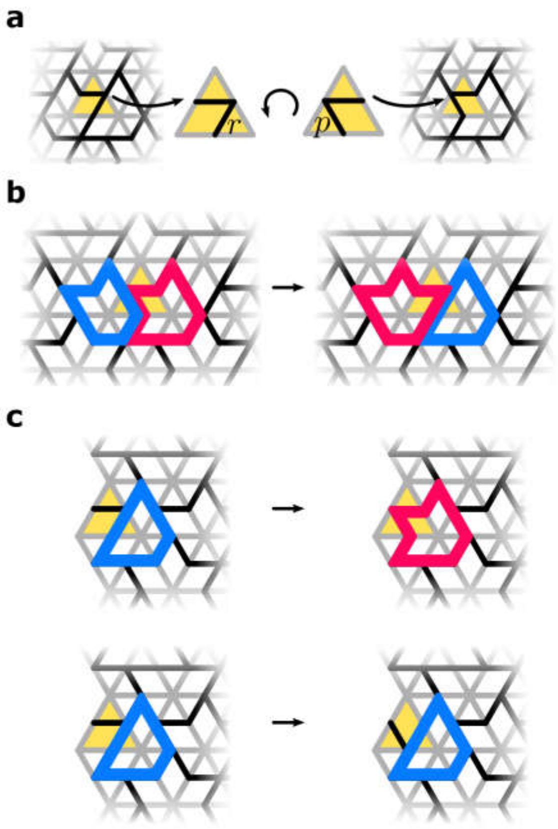

Fig. 2.11.: Supertriangle rotations transform one design to any other. a, Selecting and rotating a single building block in an architecture modifies its structure. Effectively, the rotation replaces internal bond r by internal bond p at a previously unoccupied location. **b**, Rotating a bulk building block changes local loop parities. The building block's internal bond r is part of exactly two local loops. Replacing bond r by p changes both loops' length by one, changing their parity from even to odd and vice versa. **c**, Rotating a boundary building block changes the parity of at most one local loop. Internal bonds of building blocks at the boundary of a stack contribute to either one or no local loops (top and bottom). Removing the internal bond by rotating a boundary block then changes the parity of one or no loops, respectively.

2.4.3. A topological defect

Evidently, we can induce *local* frustration in an initially compatible stack by rotating a single building block, generating a structural defect that consists of two adjacent odd local loops. However, we show now that controlled *global* frustration may also be obtained, by constructing metamaterials containing a single odd local loop.

We generate these globally frustrated metamaterials from an initially compatible system via a sequence of building block rotations running in a chain between the desired odd local loop locus and the system's boundary. Specifically, we rotate a building block at the edge of a structural defect, ensuring that the internal bond that is removed during the building block rotation contributes to one odd and one even local loop (Fig. 2.12b-c). As before, the rotation changes the parity of the two local loops. Consequently, the two odd local loops of the original structural defect are no longer adjacent after the transformation: they are now separated by a single even local loop (Fig. 2.12c). This defect configuration, consisting of two incompatible superhexagons separated by one or more compatible ones, can no longer be removed by a single, local building block rotation. To finally obtain a single odd local loop, we repeat the above procedure to displace one of the two odd local loops closer and closer to the system's boundary. Finally, we select a boundary building block that contributes to exactly one odd local loop, so that its rotation causes that odd loop's parity to become even (Fig. 2.12d). One of the two odd local loops is thus 'annealed' out of the network via the boundary via a series of building block rotations—as an aside, it is therefore not possible to create single odd local loops in networks under periodic boundary conditions.

The procedure shown in Fig. 2.12a-d leaves us with an isolated odd local loop in the system's bulk, that can only be removed by an extensive number of building block rotations that involve the network boundary. In addition, all loops of internal bonds that circumscribe the isolated odd local loop are now of odd length. Thus, the parity of loops around the system's perimeter fundamentally differs in the presence of a single odd local loop. We therefore refer to the odd local loop as a *topological defect*[26,27] which affects the metamaterial at the global scale.

We note that, in contrast to defects occurring in metamaterials where the nontrivial topology results from a nonzero winding number in momentum space[17,18,44], here the topological character of defects is governed by the parity of real-space local loops.

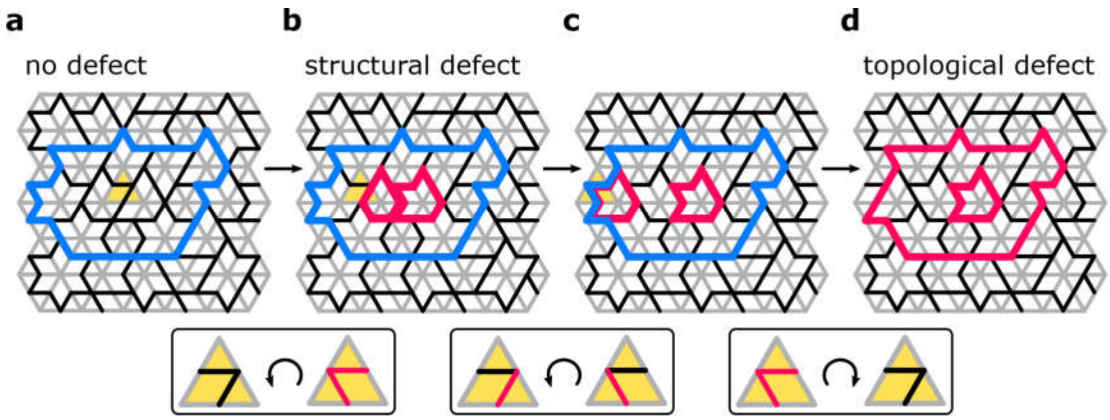

Fig. 2.12.: Generating frustration with a local or a global character. **a**, A compatible network design where all loops of internal bonds, such as the highlighted blue circuit, are of even length. **b**, Rotating a single building block (yellow triangle, inset) generates two adjacent odd local loops (red lines). These form a structural defect that frustrates the compatible motion of the material. Larger loops around the system boundary remain of even length. **c**, The adjacent odd local loops are moved apart by selecting and rotating another building block (yellow triangle, inset). The transformation generates two isolated odd local loops, separated by an even local loop. System boundary loops remain even. **d**, A final rotation removes one of the odd local loops from the material. A single topological defect remains. Its global character is felt at the system boundary: loops of internal bonds around the network edge now have odd length, signifying global frustration.

2.4.4. More odd local loops

Complex sequences of block rotations can produce more than only one or two odd local loops. Higher numbers of odd local loops can be classified to have a local or global character: in a network with an even number of odd local loops, internal bond loops around the system perimeter are of even length, showing a breakdown of compatibility that is locally confined to the material's bulk. Conversely, an odd number of odd local loops produces odd loops around the system perimeter, signifying global frustration that involves the system's edge. The parity of the number of odd local loops is therefore an order parameter that signifies the local or global character of frustration in the network, as measured around the system's boundary.

2.5. Conclusions and outlook

Our work shows how sufficiently complex building blocks can be combined into an extensive number of compatible metamaterial designs. Such compatible metamaterials contain only closed loops of internal bonds with even length, which ensures the presence of a floppy, zero-energy deformation mode.

We include targeted, discretely controlled frustration and nontrivial topology in our metamaterials by introducing odd loops of internal bonds. Such odd loops signify frustration of the material's floppy mode: two adjacent odd local loops constitute a structural defect with a local character, while an isolated odd local loop constitutes a topological defect with a global character.

More generally, our strategy opens up a new avenue for studying topological, spatially complex states in artificial materials that are experimentally accessible[45]. In the following chapters, we accordingly study the mechanics of our complex mechanical metamaterials, focusing on the distinct mechanical signatures of structural and topological defects.

Acknowledgements

This work was performed in close collaboration with Martin van Hecke, Erdal Oğuz, and Yair Shokef. We thank Roni Ilan, Edan Lerner, Bela Mulder, Ben Pisanty, Eial Teomy and Ewold Verhagen for fruitful discussions, and Rivka Zandbergen for supplying the exact counting data in Fig. 2.6 and Fig. 2.10. This research was supported in part by the Israel Science Foundation Grant No. 968/16.