

Mixed Triangular-Square Lattices on a Spherical Surface

by

Han Xie

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Author's Declaration

This thesis consists of material all of which I authored or co-authored: see Statement of Contributions included in the thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Statement of Contributions

This thesis contains content that was published. The content in Chapter 2 was published in *Nano Letters* in 2025 [1]. The content was co-authored with Wenyu Liu, Zhenyue Lu, Jeff Z.Y. Chen, and Yao Li. The content in Chapters 3 and 4 was published in *Physical Review E* in 2025 [2]. The content was co-authored with Yao Li and Jeff Z.Y. Chen. In both cases, I was the first author and mainly contributed to the theory, simulation, and calculation. The manuscript was written by myself, with edits and contributions by my co-authors. Chapters 1 and 5 were solely authored by myself.

Abstract

Defects play a crucial role in determining the structures and properties of materials. When putting lattices onto a curved surface that has non-trivial Euler characteristics, defects must appear due to the geometric frustrations. Extensive studies have shown the singular lattices on curved surfaces presenting point- and scar- disclinations with high symmetry. Of recent interest is the mixed ordered lattices on flat surfaces. The phase separation of multi-ordered lattices produces a complicated, maze-like structure, where defect also plays an important role. It makes us curious about the defect properties when arranging mixed lattices on a curved geometry. In the thesis, we propose and discuss a computational and theoretical approach to study the properties of the mixed two-dimensional triangular-square lattices on a spherical surface.

First, we introduce Hertzian interactions in molecular dynamics simulations to stabilize the coexistence of triangular and square domains and enable soft particles to self-assemble on a sphere. The simulations reveal novel defect morphologies beyond conventional point and scar defects—domains of one lattice type acting as defects within the bulk of the other, arranged with unexpected symmetry.

To analyze these assemblies further, we develop tiling methods to arrange mixed triangular-square lattices onto spherical geometries, where defects type and locations are determined. we generalize the Caspar–Klug construction for triangulations of the sphere and introduce two operations—Face-Rotation (FR) and Cut-and-Rotate (CR)—to generate mixed tilings with minimal defects and high symmetries.

This tiling methods enables the comparison of the defective energies of these structures with a coarse-grained model developed by Bowick *et al.*. A state diagram is plotted to show the energetically favored structure at a given area fraction of square lattices. Finally, we compare these mixed configurations to singular lattices via a limiting approximation to their energy landscapes.

Our work presents a new angle to understand the tripartite tug-of-war among crystalline orders, defects, and topology—an interplay that occurs across scales, from biomolecular assemblies to architectural frameworks.

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Dedication

This is dedicated to my parents X.H. Xie and H.M. Deng, who unconditionally support.

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Chapter 1

Introduction

Lattice theories serve as essential frameworks in condensed matter physics, chemistry, and even biology, governing the organization of atoms, molecules, or larger building blocks in diverse materials and complex assemblies. Their structural integrity and symmetry underlie a range of fundamental properties, including electronic band structure, phonon spectra, optical characteristics, and mechanical stability, thus playing a pivotal role in shaping modern scientific understanding of matter [5]. The concept of organized, repeating structures can be traced back to the early work of Johannes Kepler on close packing in the 17th century [6] and was formalized in the 19th century by Auguste Bravais, who classified crystal lattices into distinct symmetry groups [7]. Studies of flat (Euclidean) lattices have accordingly flourished, leading to extensive insights that drive advances in crystallography, solid-state physics, and materials science. In this chapter, we present a survey to highlight the pathway of lattice theories that leads to our research on coexistent lattices in curved geometries, where curvature and phase separation of multi-ordered lattices introduce striking new effects absent in Euclidean space.

1.1 Defects

Understanding the physical origin of defect features is essential in materials science. In crystalline and ordered systems, perfect periodicity is idealized. However, in real systems, various defects occur that strongly influence the physical and chemical properties of materials. Even though these imperfections typically take a small fraction of the total structure, they can play a decisive role in material properties.

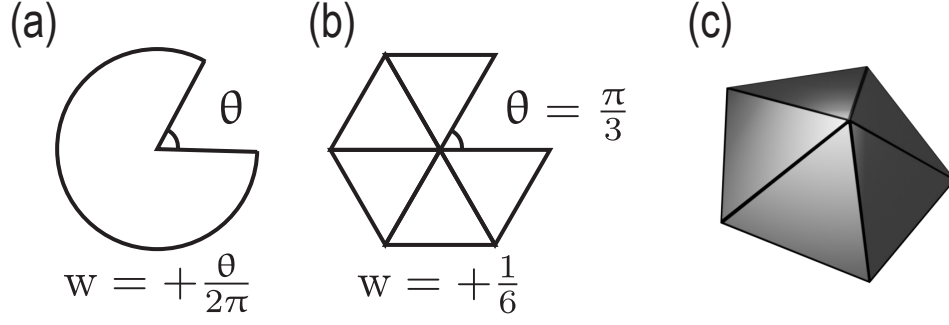


Figure 1.1: (a) and (b) Schematic illustration for the definition of winding number. (c) Illustration for the “out-of-plane” effect of disclinations.

Defects can be categorized into two groups. The first group is referred to as point defects, including vacancies, interstitials, and substitutions. Vacancies are missing atoms in lattices; interstitials are extra atoms that occupy spaces between the regular lattices sites; substitutions are foreign atoms replacing host atoms. Such defects can alter material properties like electrical conductivity and diffusion rates. For example, doping a semiconductor by introducing substitutional atoms is a common method to control its electronic behavior [5, 8, 9]. However, this group of defects is less relevant in this work. The reason is that point defects, being local in nature, do not significantly affect the global symmetry or stress distribution of the system. Therefore, while they can influence certain material properties in flat or weakly curved geometries, they play a negligible role in the curvature-driven phenomena and defect morphology explored in this study.

The second group is referred to as topological defects, including deformation, dislocations, and disclinations. These three types of defects usually do not involve foreign atoms. Instead, they cause long-range influence on the material. The presence and distribution of the topological defects are central to material properties such as the elasticity and strength of metals, or the conductivity of semiconductors [10].

Deformations are smooth, continuous distortions of the lattice that slightly bend or stretch it without breaking the overall pattern. They help the structure adapt to the curved surface by slightly shifting the positions of its components.

Dislocations occur when there is an extra row or a missing row of atoms or particles. In a curved surface, this mismatch acts like a “seam” where the lattice adjusts to the curvature by shifting the regular arrangement along a line.

Disclinations are defects where the local rotational order is disrupted. One can picture this by removing a slice from a circular pizza and then trying to reassemble the remaining

slices into a complete circle, as in Fig. 1.1(a). To close the gap, the slices must be rotated slightly out of alignment, resulting in a small angular mismatch and a stretch deformation along the outer edge of the slices. On a flat surface, the energy cost of forming a disclination is high because it induces long-range deformations throughout the bulk. However, by lifting the central point of the "pizza" out-of-plane, the remaining slices naturally close the gap without stretching their edges, forming a pyramid, as in Fig. 1.1(c). This example illustrates how disclinations reconcile curvature, naturally introducing out-of-plane displacements into an otherwise flat lattice.

When the regularity of lattices is disrupted by curvature, the topological defects play an important role. Among them, the disclinations are considered the most critical, and as a core part of our study. In the context of lattice disclinations, the winding number is a way to characterize the intensity of disclinations, by measuring how much the local orientation of the lattice "rotates" as you go around the disclination. In a perfect, defect-free lattice, if you complete a full circle, the orientation of the lattice returns to its original state with a total rotation of 2π . However, when a disclination is present, the lattice is disrupted, and the cumulative rotation might be less or more than 2π . Thus, the winding number tells how many fractions of a full rotation the lattice misses (gains).

The value of winding number is defined as follows: if the lattice rotation around a disclination misses θ than 2π , the winding number of this disclination is defined as $w = +\theta/2\pi$. In reverse, if the rotation gains θ , its winding number is defined as $w = -\theta/2\pi$. A schematic illustration of winding number calculation is shown in Fig. 1.1. In simple terms, the winding number for a disclination quantifies the angular mismatch introduced by the defect, helping to understand and classify how the lattice is deformed around the defect. The sum of the winding number of disclinations in a system equals the Euler characteristic $\chi = V - E + F$, where V , E , and F are respectively the numbers of vertices, edges, and faces in the given topology [11]. For example, $\chi = 2$ for a convex polyhedron and for spheres.

In the following sections, we will demonstrate why topological defects are essential in systems with curved geometries and mixed crystalline orders.

1.2 Lattices on curved geometries

Continuous advances in the study of lattices have inspired a broad spectrum of related research. Since the 1950s, studies of viral capsids have highlighted the profound role of geometric frustration in lattices, where proteins self-assemble on curved surfaces such as

cylinders and spheres. Experimental results such as X-ray diffractions show the spherical virus found in nature has a high symmetry configuration, with triangular building blocks. To study this topic, lattice structures on curved geometries have started to attract attention.

Initially, in 1957, Crick and Watson proposed that spherical viruses were composed of 60 identical triangular subunits, arranged with icosahedral symmetry (a polyhedron with 20 identical faces) [12]. However, experimental findings later revealed that many viruses contain a different number of subunits. To resolve this discrepancy, Caspar and Klug proposed, in 1962, a method for constructing triangular lattices on a spherical surface [3]. According to their work, if the number of particles N satisfies $N = 10(n^2 + nm + m^2) + 2$, where n and m are integers, the spherical surface can be perfectly tiled with a triangular lattice that exhibits icosahedral symmetry. This construction results in the presence of twelve pentagonal disclinations (each with a topological charge $w = +1/6$ and composed of five triangles) located at the vertices of the icosahedron [see Fig. 1.1(b) and an example in Fig. 2.3(a)]. The triangular lattice can subsequently be substituted with subunits that possess either 3- or 6-fold symmetry, effectively explaining the structures of spherical viruses.

Moreover, the Caspar-Klug construction not only deepened the understanding of viral architecture but also opened up a vast playground for research in biology, physics, chemistry, materials science, and even architecture. A subsequent milestone in this area was the discovery of fullerenes—most notably the Buckminsterfullerene C_{60} [13]—which revealed that constructing a spherical carbon lattice predominantly composed of hexagonal rings necessitates the introduction of exactly 12 pentagons. Additionally, various icosahedral virus structures, consisting of protein blocks in different shapes, have been revealed [14, 15]. Icosahedral protein cages and capsules are designed and manufactured [16, 17], for industrial, pharmaceutical, and scientific uses. The construction method for spherical triangular lattices also finds applications in soft materials [18, 19] and crystalline solids [10, 20].

Later, researchers examined the energetic relationship between defects and curvature. In the 2000s, Nelson and Bowick demonstrated using elastic theory that topological defects, particularly disclinations, form on curved surfaces [21]. They showed that disclinations behave similarly to electric point charges: a $+w$ disclination acts like a $+q$ charge, while a $-w$ disclination acts like a $-q$ charge. Creating a disclination on a flat surface requires a large amount of energy. Disclinations with the same sign repel each other. Furthermore, a curved surface with curvature K behaves like a plasma with a charge density. For instance, a sphere with constant positive curvature is comparable to an electric plasma with negative charge density. As charges in a plasma screen each other, disclinations can

effectively cancel each other’s effects. This explains why a positive $+w$ disclination tends to appear on a surface with positive curvature $+K$, and why twelve disclinations on a sphere usually spread out evenly, forming an icosahedral pattern. In 2002, Bowick and Nelson predicted that a single disclination cannot effectively screen curvature as the area increases, leading to the emergence of dislocations that help reduce the system’s energy [21]. In triangular lattice systems, a single dislocation consists of a dipole formed by two opposite disclinations — a 5-fold disclination with a winding number of $w = +1/6$ and a 7-fold disclination with $w = -1/6$. Although their combined winding number is zero, they inserting an extra row of atoms helps relieve the deformation nearby. These dislocations connect to the original point disclination and form a characteristic 5-7-5-7-5 structure, which looks like a scar separating two regions of the regular lattice [see Fig. 2.2(b)]. This type of scar was later confirmed experimentally in 2003 through the assembly of colloidal beads on the surface of a liquid droplet [22]. Overall, their energetic perspective and the identification of scar defects provide a valuable extension to the Caspar-Klug construction.

In parallel, Lubensky, Vitelli, and others made significant contributions by applying continuum elasticity theory and topological considerations to liquid crystals and membranes on spherical geometries [23, 24, 25, 4], further elucidating how curvature-induced stresses drive defect formation and organization. This body of research unifies disparate systems—ranging from spherical liquid crystals and colloidal assemblies on droplets to biomolecular shells—revealing that the universal interplay between elasticity, topology, and curvature underlies various defect patterns in various systems.

In recent years, researchers have begun exploring lattice formation on geometries more complex than spheres, such as ellipsoids, hyperboloids, and tori—revealing an even richer landscape of defects and topological constraints [26, 18, 27, 28, 29]. Moreover, defects have been investigated in more experimental systems. Examples include confined molecules or polymer beads ($\sim 10\mu\text{m}$) on spherical droplets formed by water-oil emulsions that display local hexagonal crystalline order [22, 30, 31, 32], the assembly of divalent nanoparticles [33] that exhibit polar order [34], the structure of double emulsions of liquid-crystal droplets ($\sim 10\mu\text{m}$) [35] that contain local nematic order [36, 37]. It is also believed that surface structural morphology is linked to the functionality of biological matter, such as virus shells which display both hexagonal [14] and square lattices made of proteins ($\sim 10\text{nm}$) [38, 39], bacterial surfaces [40] and vesicles made of lipids ($\sim 10\text{nm}$) [41, 42], as well as engineered cages formed by protein assembly [43, 44].

Taken together, these efforts underscore the universality of geometric frustration: from viruses and carbon nanostructures to soft matter and synthetic self-assemblies, curvature and topology dictate both the stability and the peculiar spatial arrangement of defects in ways beyond traditional crystallographic frameworks. These studies have also guided

practical developments in industries and pharmaceuticals, where controlling curvature-driven self-assembly can lead to new drug delivery systems, advanced materials, and other innovative applications [18].

1.3 Mixed lattices

Research on lattice has also branched out into mixed lattices, where two or more ordered lattices coexist in a system. Unlike a single ordered lattice on a flat surface that exhibits translational and rotational symmetries and can tile an infinite domain, the coexistence of distinct lattice phases presents additional complexities. These arise from factors such as interfacial mismatches, competing symmetry requirements, and the formation of defects, all of which can significantly alter the material’s overall properties. Researchers have looked into the crystalline-crystalline coexistence, bridging knowledge from classical metallurgy to novel colloidal crystals with tunable interactions. In metallurgy, for example, multiple grains with different crystallographic orientations often meet at grain boundaries, whose structure and properties affect both mechanical strength and material performance [45, 46, 47]. Meanwhile, in “super-ice” phases observed at high pressures or low temperatures, regions of structurally distinct ice polymorphs can coexist, giving rise to unique interfacial phenomena [48, 49]. Colloidal systems with precisely tunable interparticle potentials provide yet another platform where lattice coexistence emerges, stabilized in some cases by disclinations and dislocations that accommodate mismatches in lattice spacing [50, 51, 52]. These colloidal systems are also observed via experiments [53, 54].

Unlike common liquid-liquid or liquid-gas phase separation that are governed primarily by enthalpic and entropic considerations, the elastic strain energy in lattice-lattice coexistence plays a central role in determining global structure. Because the lattice constants and symmetries differ at the interface between two coexisting phases, topological defects are required to bridge the mismatch [55, 56], thus enabling both lattices to maintain stability. This phenomenon has been verified by a range of experimental and computational studies, underscoring how the interplay of elasticity, topological defects, and microscopic forces collectively dictates the formation, stability, and morphology of coexisting lattice phases [10, 52]. Additionally, theoretical frameworks have been given for a generalized multi-phased lattices equilibrium [57].

Conclusively, coexisting lattice phases on flat substrates, governed by elastic strain energy and mismatch-driven topological defects, yield complex structures with critical implications for industrial materials, advanced manufacturing, and emerging technologies [58].

1.4 Outline of the paper

As illustrated above, we recognize that topological defects play a crucial role in both lattices on curved geometries and mixed lattices on flat surfaces. This naturally raises the question: What kind of structures emerge when lattices are mixed on curved surfaces, and how do defects affect coexisting lattices under such conditions? Surprisingly, we have found no previous work that directly addresses this issue.

In this paper, we seek to explore coexisting lattices on curved geometries, beginning with the simplest curved surface—a sphere of constant curvature. We select triangular and square lattices, two highly symmetric and widely observed lattice types as the two lattice types in our crystalline coexistence. Although real surfaces are often quasi-planar and allow for multilayer arrangements, here we simplify the analysis by restricting particles to a strict two-dimensional single-layer configuration. This approach makes it easier to observe and characterize the resulting structures.

Taken together, our investigation is the mixed triangular-square lattices on a spherical surface, proceeding along three complementary perspectives:

1. Computer simulations (Chapter 2),
2. Tiling methods (Chapter 3),
3. Elastic theory (Chapter 4).

In Chapter. 2, we wish to directly observe the structures of spherical mixed lattices. We choose computer simulation because we have limited prior knowledge of the systems. We begin by adopting a specific Hertzian inter-particle interaction that can stabilize coexisting triangular–square lattices under suitable physical conditions, together with a simulated annealing algorithm to self-assemble particles on spherical surfaces. We find that unlike single-ordered spherical lattices that primarily exhibit point disclinations, and crystalline-crystalline phase separation on flat surfaces that display shortest boundaries, phase separation of two ordered lattices on spheres generates small domains of one lattice type that act as defects in the bulk of the other. These “domain-defects” form structures with global symmetries such as octahedral, tetrahedral, and hosohedral. Even more striking, we observe “counter-domain defects,” in which a smaller domain of one lattice lies within a larger domain of another, effectively functioning as a domain-defect in the first lattice’s bulk. These complex architectures arise from the combined influence of lattice competition and geometric frustration.

In Chapter 3, based on the structures observed from simulations, we develop a tiling method to list all spherical defective structures with mixed triangular-square lattices that have high symmetry. This method is inspired by Caspar and Klug’s construction for spherical triangular tiles. We begin with the Platonic solids, polyhedra with one type of face, because they offer the highest symmetry in each point group. Platonic solids include the icosahedron, cube, octahedron, tetrahedron, and others. We find that the truncated versions of these solids, in which the sharp corners are sliced off and replaced by flat faces, are optimal for tiling mixing lattices while producing the fewest defects. These tilings display the full symmetries of octahedral (O_h), tetrahedral (T_d), and dihedral (D_{Nh}). From these symmetric classes, we introduce an operation called Face-Rotation (FR) in which all truncated faces are rotated by a certain angle, making the lattices in the bulk rotate as well and does not disrupt the lattices arrangements, thereby breaking the reflective symmetry. In addition, some symmetric classes include an equatorial plane that divides the sphere into two hemispheres with identical lattice orientations along the boundary. This arrangement allows us to rotate one hemisphere and reattach it without altering the boundary tiling, an operation we refer to as Cut-and-Rotate (CR). Both FR and CR expand the range of full symmetric tilings to include classes with lower symmetry, a finding similar to those in spherical systems of protein clusters, liquid crystals, and lattices.

Finally, in Chapter 4, we wish to compare the energies of the various classes obtained in Chapter 3. Given a symmetry class, the area fraction of square lattices, as well as the parameters for specific FR and CR operations, the locations of defect points on the sphere are determined. Although no microscopic details are provided, the elastic energy caused by defects can be calculated by a coarse-grained model developed by Bowick et al. [18]. The Bowick–Nelson–Travesset (BNT) model estimates the defect energy on spherical surfaces based solely on defect positions, treating disclinations as repulsive charges interacting via a geodesic-distance-dependent potential. By systematically constructing configurations with varying area fractions and FR/CR angles, we generate a phase diagram that identifies the minimum-energy structures among the previously discovered symmetry classes. Furthermore, we explore the limiting case where the area fraction of one lattice approaches 1, allowing us to compare the defect energy landscape of single-lattice configurations under FR and CR operations—a regime often inaccessible to purely continuum approaches.

Given the wide application of spherical triangular lattices in fields like virus structure and nanomaterials, our work on coexisting triangular–square lattices on spherical surfaces may offer new insights. By using computer simulations, tiling methods, and elastic theory, we show that lattice competition and geometric frustration lead to complex defect patterns such as domain and counter-domain defects. These results not only help us better understand how defects form in curved crystals but also point to practical uses in design-

ing advanced materials, nanostructures, and devices where controlled defects can improve performance.

Chapter 2

Computer Simulation

Computer simulations offer an effective way to explore systems with limited prior knowledge. For studying soft matter, such as colloids, polymers, and liquid crystals, computer simulation allows researchers to explore the microscopic behavior and interactions of these systems without needing extensive or expensive experiments. Methods like Monte Carlo simulations, molecular dynamics simulations, and Brownian dynamics simulations help capture the complex behavior of soft materials, from self-assembly to phase transitions [59].

To elucidate how spherical geometry affects single-layer mixed triangular-square lattices, in this chapter, we provide a physical picture of the structural formations on the spherical surface by computer simulation with the Hertzian interaction potential, which enables a stable triangular-square lattices coexistence, meanwhile having a soft repulsion core below the interaction range to capture the elastic nature between colloidal particles [50, 60, 51, 52].

Through extensive computer simulations of systems containing a large number of soft particles in various packing densities, rich structural configurations are discovered near the triangular-square crystalline-to-crystalline transition density. The existence of domain and counter-domain defects is revealed, which were rarely discussed in the literature. The competition between triangular- and square-lattice stabilities near the crystalline-crystalline transition point enables rectangular defect domains (rich in square tiling) in a triangular-tile background, and triangular defect domains (rich in triangular tiling) in a square-tile background. The compound winding numbers as a complete unit of a domain defect make the entire system arrange the defect locations differently from those of point or scar defects.

More surprising is the emergence of counter domains when triangular and square tiles have comparable area fractions, and the defect domains occupy a large surface area. The

edges between the hosting defect domain and the background lattice are substantially curved, forming a spherical polygon (biangle, triangle, etc.), which has a larger sum of internal angles than its flat-space counterparts, a typical consequence of the Gauss-Bonnet theorem. Neither triangular- nor square-tiles can uniformly fill the host domain area without creating lattice mismatches. Then, enclave counter domain defects appear within the host domain defects.

2.1 Simulation method and winding number

The simulation is performed using Hertzian interaction, which is purely repulsive. This interaction has become the choice in computer simulations [50, 60, 51, 52], modeling the stability of triangular, square and quasi-crystals when colloidal particles are closely packed. It has also been successfully used to model the experimental results of soft microparticles in a flat two-dimensional plane [61] or a three-dimensional space [62], unraveling the physical insights behind the real systems.

Between two soft colloidal molecules, labeled j and k , which have the center-of-mass coordinates $\mathbf{r}_j$ and $\mathbf{r}_k$, the interaction follows [see Fig. 2.1(a)],

$$U(r_{jk}) = \begin{cases} \varepsilon (1 - r_{jk}/\sigma)^{5/2}, & \text{when } r_{jk}/\sigma \leq 1, \\ 0, & \text{otherwise,} \end{cases} \quad (2.1)$$

where $r_{jk} = |\mathbf{r}_j - \mathbf{r}_k|$, σ is the force range between the two, and ε (positive) the magnitude. In the current study, the centers of N such elastic molecules fill the surface of a sphere of radius R in dense packing. When the system energy reaches a minimum, the configuration of the molecules are characterized by two dimensionless physical parameters, the number of filling molecules N and the reduced overall density $\rho^* = N\sigma^2/4\pi R^2$. Though the model is overwhelmingly simple, it has been used to produce some most basic defect properties caused by the interplay between the geometry confinement and packing frustration [50, 60, 51, 52].

We employ the Rattle algorithm [63, 64] to conduct molecular dynamics of particles constrained on the sphere, where the interaction between particles are modeled by the Hertzian potential as in (2.1). The simulations are performed using simulation package LAMMPS [65]. The initial configurations of N particles are randomly generated on given density ρ^* for a given sphere radius R . Temperature T is reduced and measured in units of ε/k_B . During the simulation, simulated annealing [66] is performed slowly from temperature $T_0 = 10^{-2}$ to the target temperature $T < 10^{-4}$, according to $T = T_0 \exp(-0.002 \times n)$

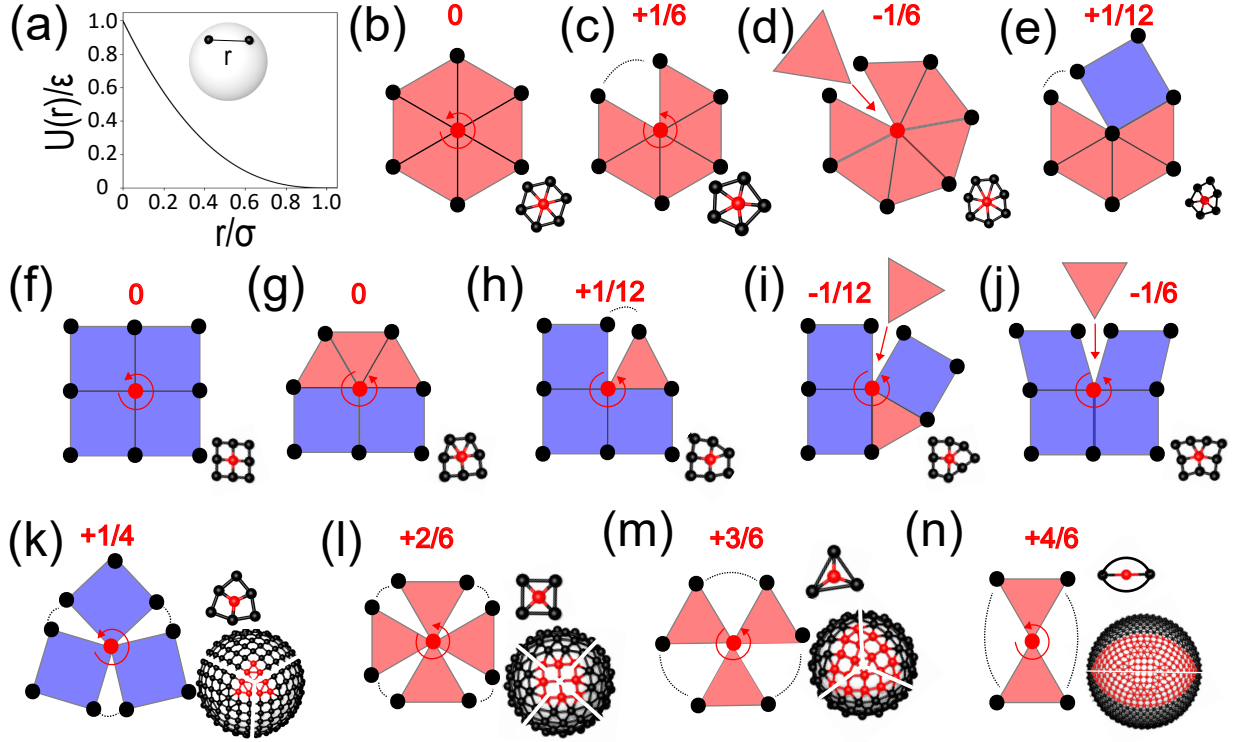


Figure 2.1: Interaction potential and disclination types. The interaction between two soft particles is modeled by the Hertzian potential in (a), where the r is the Euclidean distance. Colloid particles are confined on a spherical surface as illustrated in the inset. Plots (c), (d), (e), (h), (i), and (j) illustrate the common point-defect types observed here, where the corresponding winding numbers are shown as the red fractions. Plots (k)–(n) illustrate the domain defects discussed in the text, with their compound winding numbers in multiplicity of the basic values.

with $n = 2500$ steps. This annealing process is controlled by the Langevin thermostat with a relaxation time of $10dt$. At each temperature 5×10^4 time steps were performed. The time step of the MD simulations is set at $dt = 0.5$, in units of $\sqrt{m\sigma^2}/\varepsilon$. As the final step, the system is quenched to zero temperature by back tracking energy minimization [67].

Defect patterns observed in the simulation are listed in Fig. 2.1(b)-(n), with their corresponding winding numbers w written on top of each subplot. Disclinations found in mixing triangular-square lattices typically compose of triangle and square cells, characteristically having a denominator 6 for a mismatching triangular cell (angle $2\pi/6$) or 4 for a mismatching square cell (angle $2\pi/4$). The preceded sign of the winding number is a description of a missing lattice cell (+) or an inserted lattice cell (−). A winding number with a denominator 12 corresponding to the simultaneous addition of a triangle cell and removal of a square cell [a net $-1/6 + 1/4 = +1/12$, see pattern (e) and (h)], or vice versa [a net $-1/12$, see pattern (i) in reference to (g)]. Multiple removals of triangle cells can produce a winding number in multiplicity of $1/6$; examples are patterns (l), (m), and (n). All defects observed in our study follow this formula with the total summed w of $\chi = 2$, the Euler characteristic of the spherical surface [11].

2.2 State diagram and defects

Figure 2.2(a) illustrates the state diagram found from our study, of relatively large systems ($N \geq 750$). To find the ground states, we performed independent 20 simulated annealing simulations for each of the 840 uniformly distributed sampling points in the state diagram; among these, the states having the lowest energies are chosen and analyzed.

As density increases from $\rho^* = 1.9$ to $\rho^* = 2.7$, the dominating order in the system transitions from triangular to square lattices, as can be characterized by the bond parameter ϕ_p :

$$\phi_p = \frac{1}{Np} \sum_{j=1}^N \left| \sum_{k=1}^p \exp(ip\theta_{jk}) \right| \quad (2.2)$$

where p neighbors nearest in distance, labeled k , are used for molecule j . One can show that for an ideal triangular lattice $\phi_6 = 1$, and square lattice, $\phi_4 = 1$, while the other ϕ_p -values are significantly smaller. Hence ϕ_p is the bonding order parameter of a p -fold lattice [68]. On the spherical surface, due to topology frustrations, both triangular and square lattices, or even a mixing of the two types of lattices, accompany defect points, scars, and domains; hence ϕ_4 and ϕ_6 never reach the idealized value of 1. On the top panel of Fig. 2.2(a), ϕ_6 monotonically decreases, and ϕ_4 increases as density increases.

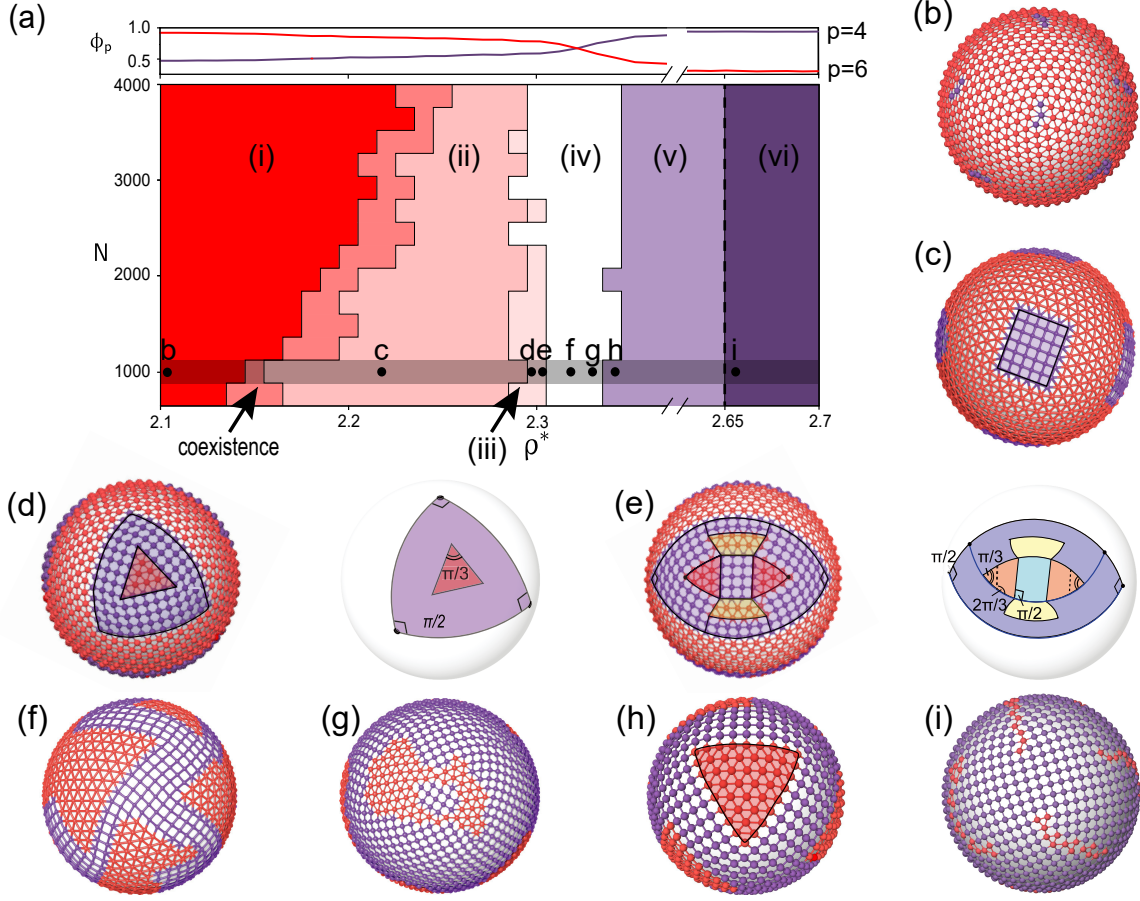


Figure 2.2: State diagram of the Hex-Sq coexistent region and simulation snapshots. Six main regimes, (i) to (vi), are observed from our computer simulations of the Hertzian potential, depicted in (a). The upper panel of (a) displays the overall lattice order parameter ϕ_4 and ϕ_6 for $N = 1000$. The lettered locations in the state diagram (b-i) are where the snapshots in (b) to (i) are taken. In regime-(i), deformed Hex lattices on spherical surface contain either localized point disclinations or scars [plot (b)]. In regime-(ii), Sq-lattice domains appear in the background of deformed Hex lattices [plots (c)]. In regime-(iii), enclave Hex-lattice domains exist inside Sq-lattice domains, which are embedded in the background of deformed Hex lattices [plots (d) and (e)]. Regime-(iv) contains significant Hex- and Sq-lattice domains interwind together, where no clear global symmetry can be detected [plots (f) and (g)]. In regime-(v), localized Hex-lattice domains exist in a majority of Sq-lattice domains [plot (h)]. Beyond that, in (vi), the spherical surface is covered by deformed Sq lattices containing isolated point or scar disclinations [plot (i)]. In between i and ii, coexistence of the structures seen in i and ii is observed.

The crossover occurs around $\rho^* \approx 2.35$. In a flat space, in the thermodynamic limit, one can show that the uniform triangular lattice is stable when $\rho^* < 2.255\dots$ and square lattice when $\rho^* > 2.364\dots$, theoretically. In a previous computer simulation, the crossing of ϕ_6 and ϕ_4 , at $\rho^* = 2.228$, is thought of as the first-order triangular square phase transition point [52]. On a spherical surface, all interesting regimes appear near these densities.

Based on the defect patterns and other disclination properties discussed below, six distinct regimes are obtained: (i) the surface is covered by a single, deformed triangular lattice with point disclinations [Fig. 2.2(b)] or scars; (ii) the triangular-rich background encloses square-lattice domain defects [Fig. 2.2(c)]; (iii) the square-lattice domain defects in (ii) further enclose triangular-rich domain defects [Figs. 2.2(d) and (e)]; (iv) non-symmetric patterns where triangular-rich and square-rich domains are phase-separated [Figs. 2.2(f) and (g)]; (v) square-rich background containing scattered triangular domain defects [Fig. 2.2(h)]; and (vi) a single, deformed square-lattice background hosting point or scar disclinations [Fig. 2.2(i)].

The configurational properties described below can be repeatedly confirmed from the simulations of all regimes. The boundary between regimes-(i) and (ii) is not a clear line division; in a narrow corridor both types of defect patterns can coexist with comparative system energies. Along the dashed boundaries, coexistence of the nearby states is also observed, but in very narrow density ranges.

The smaller systems ($N \lesssim 750$) of competing lattices display distinct, finite-size behavior, as the particle number fluctuations significantly affect the morphology of the minimum energy structure. In Ref. [50], defect structures up to $N = 12$ were classified for Hertzian molecules on the spherical surface, which are all repeated and verified here. Some additional, small- N structures are provided in Section. 2.5.

In triangular-rich regime-(i), 12 point or scar disclinations, each of winding number $w = +1/6$, display an overall icosahedral symmetry, expected by the Caspar-Klug [3] and Bowick [21] construction of triangular and pentagonal lattices on a spherical surface. Conversely, regime-(vi) is dominated by a defect structure where an ocean of square cells hosts eight defect domains rich in triangular cells or eight scars, of a net $w = +1/4$. These eight defects form the corners of an anti-cube. See respective examples in Figs. 2.2(b) and (i).

In the following section, the defect properties in crystalline-crystalline coexistence regimes (ii)-(v) are examined.

2.3 Shape frustrations, domains, and counter domains

In regimes (ii)-(v), triangular and square domains both occupy comparably large surface areas, preferred by phase separation. The curvature effects on the boundaries then become significant. Some display maze-like mixing, interwinding triangular and square rich bands without well-defined domains [e.g., Fig. 2.2(f)], and others counter domains, where one type of lattice resides inside a domain of another type of lattice that by itself is a defect of a larger background lattice of the first type. The existence of the maze-like, connected structures was recently observed in experiments of suspending molecules [32] and growth of two dimensional rigid colloidal lattices [31] on the spherical surface of droplets.

The separation between domains rich in triangular and square lattices is commonly observed in regimes (ii), (iii), and (v) of the state diagram. Typically, patches of localized square lattice domains appear in regime-(ii), in the background of triangular tiles, where within the relatively flat local area, the domain boundaries mostly follow straight lines [see Fig. 2.2(c)]. Four point disclinations illustrated in Fig. 2.1(e) occupies the vertices of the rectangular domain. The overall $4 \times (+1/12) = +2/6$ is then the winding number of a rectangular domain of square lattice in the triangular background, a defect as illustrated in Fig. 2.1(l). Six such rectangular domains are needed in a spherical system to have winding numbers summed to the Euler Characteristic $\chi = 2$. An idealized structure is shown in Fig. 2.3(c) for $N = 122$ and $\rho^* = 2.27$, where six such square domains are located at the vertices of an octahedron, which maximize the distances from each other on spherical surface.

In regime-(v), now of higher ρ^* , where square order becomes dominated with larger area fractions, localized equilateral-triangle domains of triangular lattice are formed with rather straight edges. An example can be seen in Fig. 2.2(h), for $N = 1000$ and $\rho^* = 2.35$. Three point disclinations [Fig. 2.1(h)] occupies the vertices of the triangular domain. The overall triangular domain hence carries the winding number $3 \times (+1/12) = +3/12$ collectively. The domain has effect to the bulk square lattices as a $w = +1/4$ defect shown in Fig. 2.1(k). Eight triangular domains exist, forming the corners of a cube. In other examples, the eight triangular domains can also display twisted-cube formation on the spherical surface [Fig. 2.3(k)].

In regime-(iii), where triangular and square lattices occupy comparable area, the emergence of counter domains is a remarkable phenomenon that highlights the competition between crystalline order and curvature. In the first example, the structure in Fig. 2.2(d), a small localized triangular lattice domain embedded in a hosting larger square-tiled triangle, which is in the background of triangular tiles. The three curved edges of the hosting domain trace out a winding number $w = 3 \times (+1/6) = +1/2$ as illustrated in Fig. 2.1(m),

which must be accounted for by the disclinations within. The three corners of the spherical triangle are where the square lattice meets the triangular lattice, three disclinations [Fig. 2.1(e)] giving rising to a domain winding number $3 \times (+1/12) = +3/12$. The small, enclave triangular lattice domain of triangular shape have three vertices where triangular lattice meets the square lattice, three disclinations [Fig. 2.1(h)] contributing the remaining $+3/12$. The next example, Fig. 2.2(e), a typical metastable state observed at $\rho^* = 2.30$, demonstrates that the shape frustration can yield an even more complicated domain morphology, where where not only an enclave domain exists, but another domain is further embedded inside. The spherical lune shape shown in Fig. 2.2(e) extends a large area. In the middle sit a localized square tiled rectangle, surrounded by two triangular tiled triangles at two opposite sides, and two triangular tiled trapezoids at the other two sides. The complex is embedded in a square tiled lune shape, in the background of triangular lattice. The texture of the background triangular lattice contributes to each of the two edges a winding number $+1/3$, making the entire outer evaluation path in the triangular region having a total $2 \times (+1/3) = +2/3$ winding number, which can be understood by Fig. 2.1(n). The two corners of the biangular shape and the six corners of the triangular counter domain all contribute $+1/12$ to this required winding number. The four-domain complexes in Fig. 2.2(d) (three are blocked behind) form a tetrahedron symmetry on the spherical surface. This particular pattern can be found in regime-(iii) in Fig. 2.2(a). The three-domain complexes in Fig. 2.2(e) are arranged around a big circle, with the same shape orientations, showing a trigonal hosohedron symmetry on the surface.

Overall, the final, global configuration that these domain structures settle down, is the manifestation of crystalline-crystallin coexistence, shape frustration, and energy minimization. It can have asymmetric domains and counter domains, some of which are illustrated in Figs. 2.2(f) and (g).

In the next section, we use the Gauss-Bonnet theorem to demonstrate the appearance of these domain defects.

2.4 Gauss-Bonnet theorem

To demonstrate that the appearance of domain and counter domains is an imperative consequence of the curved nature of the spherical surface. From geometry characteristics, the Gauss-Bonnet theorem dictates the corner angles α of n -sided polygons on spherical surface:

$$\sum \alpha = 4\pi a + (n - 2)\pi \quad (2.3)$$

where a is the area fraction of such a domain compared to the entire surface. Take the rectangular domain defect shown in Fig. 2.2(c) as the first example. Eq. 2.3 with $n = 4$ gives the summed corner angle of a spherical rectangle $(1 + 2a)2\pi$. As $a \ll 1$, the internal angle is $\pi/2$, which is suited for square tiling. And at the maximum end, if the occupied area $a = 1/6$, such a spherical square has an internal angle $2\pi(1 + 2/6)/4 = 2\pi/3$, which is an angle that can be easily tiled by two triangles. Hence, as a grows, the pattern must switch over from square to triangular tiling. The transition must happen in between $a \ll 1$ and $a = 1/6$, corresponding to six rectangular domain-defect being in a system.

The second example is the triangular domain defect shown in Fig. 2.2(h). Eq. 2.3 with $n = 3$ gives the summed corner angle of a spherical triangle $(1 + 4a)\pi$. When a is small, each of the eight triangular domains, located at the corners of the cube, has a total internal angle close to π and can be directly covered by triangular tiles. As a grows, however, the total internal angle becomes greater than π , and the triangular tiles experience more distortion to cover the area. An extreme case is $a = 1/8$; in this case, a typical internal angle of the spherical triangle is $\pi(1 + 4/8)/3 = \pi/2$; Directly adjacent to such an angle, a square tile is a better fit. Hence, somewhere between $a \ll 1$ and $a = 1/8$, triangular tiling switches to square tiling, corresponding to eight such triangle domain-defects in a system.

To conclude, depending on the area fraction of a spherical domain, the internal angles may be better suited to tilings with a specific type of symmetry, especially if minimal angular distortion is expected.

The counter-domain defects are interesting cases to be analyzed with the Gauss-Bonnet theorem. See the triangular counter domain shown in Fig. 2.2(d), for a triangle covering one quadrant of the sphere, it has a corner angle of $\pi/2$, hence the square pattern is the natural choice of tiling the near-edge interior [see the right plot of the Fig. 2.2(d)]. Though the tiling texture can endorse weak deformation moving to the central region of the domain, as the area a approaches zero, the central domain region becomes a regular triangle, where the corner angle approaches $\pi/3$, hence the system must switch to a triangle based pattern, the triangular tiling. From the physics of energy minimum, accompanying the square lattice deformation inside the spherical triangle, vertex energies begin to build up in the near-center area. The transformation to the triangular lattice releases this energy by moving the energy penalty to singular sites.

The next example, the spherical lune shown in Fig. 2.2(e) extends a large area, making $\pi/2$ biangles. As the interior of the spherical lune, having two right angles at the corner, is filled by square tiles from the edges, an intermediate spherical biangle is reached, having $\pi/3$ biangles, which is suited for the triangular tiles. Hence an enclave, triangular tiled counter domain defect must exist. Accommodating the reduction of the lunar edge lengths, two other triangular tiled domains in the middle are produced simultaneously, in consistency

with the Burgers vector formula [5]. As the central area of the spherical lune is reached, the spherical lune shrinks to a horizontal lattice line, which necessitates the existence of square lattices in the center as another level of enclave defect domain.

This scenario of defect domain, counter domain, and counter-counter domain is hence intrinsically required by the shape frustration on a curved surface.

2.5 Smaller systems

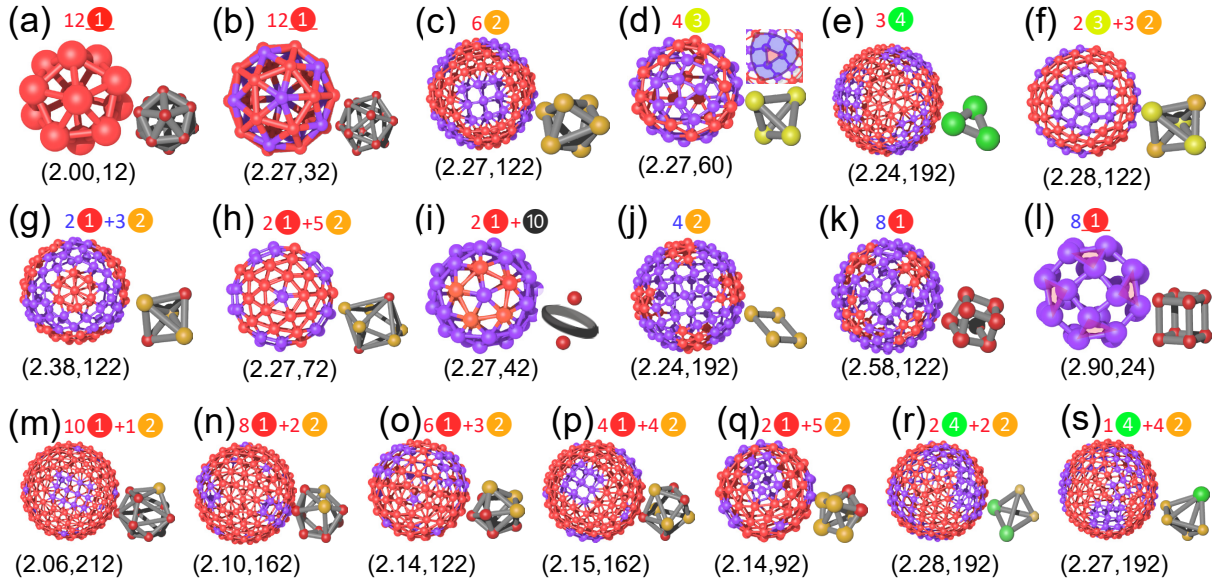


Figure 2.3: Other selective defect patterns with global symmetries. A collection of symmetric configurations are showcased in (a)-(s), adopted from the parameters (ρ^*, N) specified below the plots, for smaller N . Particles and bonds colored red are Hex-ordered and purple are Sq-ordered (including five-fold point disclination). Their corresponding spatial symmetries are illustrated in the lower right corners, rotated from the directions of the original plots for clearer presentation. In each plot, the numbers in the colored solid circles identify the defect types, prefixed by the number of defects observed in each plot.

In the previous sections, we focus on the common properties of domain defects, where global spatial symmetry can be drawn, for large- N systems. While we described these commonly occurring defect patterns by the defect “spatial symmetries” in the text, by no means they are all perfectly symmetric which only happens with selective values of N .

In small- N systems, when the triangular and square local lattices compete, the particle number fluctuation being important, insertion or deletion of a molecule into or from the system might completely revamps the defect symmetry. Shown in Fig. 2.3 are other less common defect structures, observed from the computer simulations, from the parameters (ρ^*, N) specified below the plots. Particles and bonds colored red are triangular ordered and purple are square ordered (including five-fold point disclination). Their corresponding spatial symmetries are illustrated in the lower right corners, rotated from the directions of the original plots for clearer presentation.

Every plot in Fig. 2.3 is indicated by solid circles that specify the defect types. In the triangular lattice-dominating regimes, a number n is placed inside the solid circle to represent a winding number $w = +n/6$. For example, a point disclination in the triangular rich regime is associated with $w = +1/6$ and is denoted as defect type 1. On the other hand, in the square lattice-dominating regime, a number n is placed inside the solid circle to represent $w = +n/4$. The number of defects of each type observed in a plot is indicated by the prefix on each solid circle. In the lower right corner of each plot, the configurations display the spatial symmetries of the defects, with each defect type corresponding to the same color coding as the solid circles.

Our findings are summarized below, classified by the global symmetries.

- **Icosahedral I :** The icosahedral symmetry is observed in regime-(i) of Fig. 2.2(a), where twelve point- or scar-defects occupy the vertices of an icosahedron [3]. Two extreme, minimalist examples are the $N = 12$ and $N = 32$ cases shown in Fig. 2.3(a) and 2.3(b).
- **Octahedral O :** Octahedral symmetry predominantly appears in regime-(ii) of Fig. 2.2(a), where six domain defects occupy the vertices of an octahedron, an example in small system is illustrated in Fig. 2.3(c). The octahedron pattern has also been observed in nature, when formation of square like defects is preferred [39]; and in simulation of self-assembly of Lennard-Jones particles on spheres [69].
- **Tetrahedral T :** The tetrahedral symmetry is mainly observed in regime-(iii) of Fig. 2.2(a), where four counter-domain defects occupy the vertices of a tetrahedron, as depicted in Fig. 2.2(d) and Fig. 2.3(d). Notably, Fig. 2.3(d) displays the minimal counter domain structure.
- **Tri-hosohedral C_3 :** Tri-hosohedral symmetry is observed when three defects occupy three equally spaced points on the equator, and sometime two other kinds of defects on the two poles. This symmetry is occasionally observed in small systems depending

on the particle numbers, as illustrated in Fig. 2.3(e), (f), and (g). In large systems, this symmetry is primarily seen as a metastable state in regime-(iii) of Fig. 2.2(a), which contains three counter-domain defects shown in Fig. 1(e).

- **Penta-hosohedral C_5 :** Penta-hosohedral symmetry is observed in the coexistence region between regimes-(i) and (ii) of Fig. 2.2(a). In this configuration, two point disclinations (or scar) in triangular lattices [Fig. 2.1(b)] occupy the poles of the sphere, and five domain defects form the five equally spaced points on the equator, as in Fig. 2.3(h). In smaller systems, the domain defects may assemble into a ring, as shown in Fig. 2.3(i). However, alternative configurations are possible for this defect composition, such as the asymmetric structure shown in Fig. 2.3(q). Notably, structure shown in Fig. 2.3(h) is observed in self-assembly of Lennard-Jones particles on the sphere [69].
- **square-hosohedral C_4 :** square uare-hosohedral symmetry is occasionally observed in small systems depending on the particle numbers, where domain defects locate at four equally spaced points on the equator, as illustrated in Fig. 2.3(j).
- **Cubic O :** Cubic symmetry appears mainly in regimes-(v) and (vi) of Fig. 2.2(a), where eight domain defects or square point- and scar-defects occupy the vertices of a cube. An example is in Fig. 2.3(k) for $N = 122$. The minimal example is $N = 24$ with no triangular cell, shown in Fig. 2.3(l).
- **Asymmetric:** Asymmetric structures are observed in regime-(iv) of Fig. 2.2(a), where both ordered lattices occupy comparable areas, as illustrated in Fig. 2.2(f) and (g). The structures at the boundaries of regimes with different defect compositions also often display asymmetric configurations, as shown in Fig. 2.3(m-s). Notably, the defect structure shown in Fig. 2.3(n) was also found by solving the Thomson problem, where two rectangular domain-defects coexist with eight point-disclinations [70]; and structures shown in Fig. 2.3(o) are also observed in self-assembly of Lennard-Jones particles on sphere, having lower energy than the icosahedral configurations [69].

2.6 Summary

In this chapter, we investigated the impact of a curved surface on the formation of the crystalline structures by confining N soft colloid particles on the spherical surface of radius

R. In the vicinity of the transition density, spherical areas made of triangular and square lattices have the tendency to co-exist because of the close matching in lattice energies. The curved nature of these spherical shapes introduces another level of frustration and competitions in tiling regular hexagon and square lattices. As the result, large defect domains necessitate the existence of counter domains in the interior and can even establish another level of counter domains within a counter domain. The disclination patterns discussed here combine the physics of topological defects, shape frustration, lattice energetics, and lattice tiling. Any single factor can be hardly used to explain the diversity of the observed surface features. The values of the packing densities in the current study depends on the model used; generally, the domain and counter-domain defects in real systems ought to appear between their own triangular and square stable densities.

The computer simulation of interacting particles offers a platform closely matching those in real systems. Our predictions may be realized experimentally by extending the competing triangular square lattices from planar systems [71, 72, 73, 74, 53] to spherical systems, e.g., particles confined in double emulsions [75, 76] or rounded cubes on the surface of an emulsion [77]. The topological-defect problems find their roots in other topic areas in science: for example, metallurgy [45], molecular network [78], living matter [79], and superconductivity [80]. The disclination patterns discussed here provide a unique opportunity to investigate the combined physics of topological defects, shape frustration, lattice energetics, and lattice tiling.

Recognizing that triangular-square lattices can self-assemble into various unique structures, we now wonder what other high-symmetry configurations can emerge from mixing these tilings. In the next chapter, we introduce a construction method to systematically arrange triangular-square tiles on spherical surfaces. This method builds on geometric principles and symmetry constraints to explore a wider range of configurations, potentially unveiling new classes of structures.

Chapter 3

Mixed Tiles

In the previous chapter, we conduct a molecule dynamics simulation to self-assemble mixing triangular-square lattices on a spherical surface. Although Gauss-Bonnet theorem is capable of explaining these defect patterns, we are still curious about if the MD simulation results have enumerated all the possible symmetries. If not, is there any symmetries that are neglected in MD simulation because of their energies are too high. In this chapter, we study the mixed triangular-square tiles on spherical surfaces from a geometric and symmetric angle.

As illustrated in Chapter. 1, the study of tilings on spherical surfaces has its roots in investigating the structural organization of viruses. "Placing triangular tiles to fill the surface of a sphere, what high-symmetry patterns can they form?" is the question studied by Caspar and Klug [3]. They have found that the defects on sphere typically display icosahedral symmetries, where twelve $w = +1/6$ disclinations sit at the vertices of a icosahedron. On the other hand, tiles between the defects can have different orientations, with the defect collectively presenting symmetries that characterized by point group full icosahedral I_h and icosahedral I , as noted by Goldberg who studied the geometry of polyhedron with all triangular faces [81]. By utilizing protein blocks of 3- and 6-fold symmetries, which can be nicely tiled in a triangular lattice cell, icosahedral protein cages and capsules are designed and manufactured [16, 17], for industrial, pharmaceutical, and scientific uses. The construction method for spherical triangular lattices also finds applications in soft materials [18, 19] and crystalline solids [10, 20].

The significance and widespread applications of spherical triangular tilings have aroused interest in spherical square tilings, which are also commonly found in systems of protein substrates and crystalline solids. Experimentally, stabilizing square lattices on a spherical surface is more challenging because thin-layer molecules tend to form triangular lattices in

real systems. Variations of tiling that use tetratically-shaped particles to fit the spherical surface while maintaining the local 4-fold symmetry have been explored in recent years, for example, with square-shaped protein blocks [82], rounded cube particles on emulsion faces [77], or tetratic liquid-crystal molecules [25, 4]. Analytic theories that explore the possible symmetry patterns of related systems can also be found for liquid crystals [23], square crystalline and liquid crystals [4]. Direct molecular-level computer simulations that yield local square lattices with a limited number of particles are now available [83, 20, 50]. These research indicates the spherical square tiles require eight $w = +1/4$ disclinations, sitting at the vertices of a cube or anti-cube (opposite faces of a cube rotate by $\pi/4$), depending on the physical condition of the systems. In our simulation in the Chapter. 2, single square lattices in regime-(vi) of Fig. 2.2(a) mostly display eight scar defects of $w = +1/4$, sitting at the vertices of an anti-cube. An extreme case at $N = 24$ shown in Fig. 2.3(1) have eight $w = 1/4$ triangular defects locating at the vertices of a cube. However, existing research has mainly focused on the defects' morphology and locations, the tiles between defects are omitted. We will further discuss this in Section. 3.1.2, through a symmetry analysis which also generates additional alternatives.

Then, finally, it is our question to ask: what symmetry patterns can one observe when mixed triangular and square tiles are used to cover the spherical surface? From our simulation of mixed triangular-square lattices on sphere described in Chapter. 2, we find mixed tilings display symmetries of cubic O , octahedral O , tetrahedral T , tribal-hosohedral C_3 and other asymmetric classes, as shown in Fig. 2.2 and Fig. 2.3. In addition to our research, this question is also inspired by both experimental and theoretical developments in recent years. Investigations have shown that structures formed by mixing protein block shapes with 3- and 4-fold local symmetries on spherical surfaces can exhibit octahedral and tetrahedral symmetries. These symmetries differ from the icosahedral symmetry typically observed on the surfaces of other protein complexes [84, 85, 54]. Theoretically, except for the structures found through the Caspar-Klug construction method for triangular tiles on a spherical surface, there have been no definitive answers to square tiles and mixing triangular-square tiles in the literature so far.

In this chapter, we develop a general theory to construct mixed triangular and square lattices on spherical surfaces, where the square lattice area occupies a fraction f of the surface and the triangular lattice area the remainder. A large number of tiles is assumed here and the coarse-grained continuum limit is examined. One important point to note is that the tiles considered in this chapter are designed to simulate those that emerge from local interactions or self-assembly in a large system. These tiles tend to follow coarse-grained elasticity and reflect the mechanical response of the bulk. In contrast, pre-made tiles—often rigid and immobile—are externally imposed and do not conform to the assump-

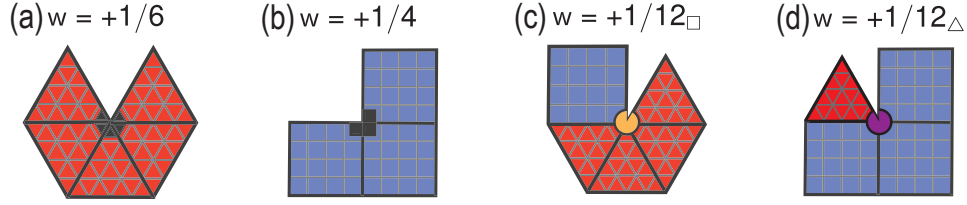


Figure 3.1: Types of point defects examined in the current study, on a spherical surface, where the flattened-out, cut views are presented. Plot (a) shows a winding number $w = +1/6$, produced by the closure of five triangular lattice domains. Plot (b) has $w = +1/4$, produced by the closure of three square lattice domains. Plot (c) is produced by inserting a square lattice domain into four triangular domains, resulting in a winding number $w = +1/12_{\square}$. Plot (d) can be viewed as the insertion of a triangular lattice domain into three square domains, with $w = +1/12_{\triangle}$. The subscripts $\square$ and $\triangle$ are used here to further distinguish the type of insertion. The color scheme of the illustrations, red for the triangular domain, blue square domain, orange defect point for $w = +1/12_{\square}$, and purple $w = +1/12_{\triangle}$, is preserved throughout the entire paper.

tions of elasticity theory. For consistency, the symmetry problems of tiling the spherical surface with only triangular tiles ($f = 0$) and only square tiles ($f = 1$) are first reviewed in Sects. 3.1.1 and 3.1.2, respectively. In the case of a fixed, nontrivial value of f , we enumerate all possible high-symmetry patterns from all Platonic Solids (polyhedron with one identical kind of polygonal face), formed by defect points and lattice texture grains. Four classes of patterns, cubic (O_h), octahedral (O_h), tetrahedral (T_d), and tri-hosohedral (D_{3h}) symmetries, are selected, listed and analyzed in Sect. 3.1.3. With one or two symmetry operations broken, kaleidoscopic alternatives, originally introduced by Caspar and Klug, are also considered in Sect. 3.2 [3], forming face-rotation (FR) alternatives of the patterns. Another possibility, known as the cut-and-rotate (CR) operation [37, 86], is additionally introduced and considered for these symmetric patterns in Sect. 3.3, forming the CR alternatives. Both alternatives preserve the lattice grains and result in lower spatial symmetries than the original O_h , T_d , D_{3h} rotational groups.

3.1 Defect patterns with the highest symmetries

In this section, possible defect patterns on a spherical surface tiled with triangular and square tiles are presented, after exhaustively searching for all possible point-group symmetries of the global patterns. Symmetry always plays a critical role in determining the

stability, organization, and physical properties of patterns on spherical surfaces, making it essential for understanding systems such as viral capsids, colloidal crystals, or geodesic domes. [18]

For clearly presenting the defects, the basic types of low winding numbers considered in this chapter are replotted in Fig. 3.1, in triangular lattices [Fig. 3.1(a), $w = +1/6$], in square lattices [Fig. 3.1(b), $w = +1/4$], and in mixed triangular-square lattices [Fig. 3.1(c) and (d), $w = +1/12$]. The subscripts $\square$ and $\triangle$ are used here to further distinguish the type of insertion. The color scheme of the illustrations, red for the triangular domain, blue square domain, orange defect point for $w = +1/12_{\square}$, and purple $w = +1/12_{\triangle}$, is preserved throughout the entire thesis. Although other point disclinations are possible, including those with higher or negative w , the point disclinations in Fig. 3.1 are commonly believed to cause the least lattice deformations on a curved surface of positive Gaussian curvature [23], hence they are considered here.

According to the Euler-Poincaré theorem, the total, summed winding numbers of all disclinations on a sphere $\sum w = 2$ [11]. Thus, there must be twelve $+1/6$ point disclinations when arranging triangular lattices, eight $+1/4$ point disclinations when arranging square lattices, and twenty-four $+1/12$ point disclinations when arranging triangular-square lattices. The locations of these defect points on the spherical surface, together with the relative orientations of the lattice domains around these defect points, form a global defect structure, which can be identified by a point group. Some different patterns may share the same point-group operations.

Deformed tiles on a curved surface may not all have an identical shape. Caspar and Klug introduced the concept of quasi-equivalence, which requires the deformed tiles on a curved surface to have nearly identical shapes in order to maintain the overall stability and functionality of the entire structure. The structures on the spherical surface can be viewed as projections of the flat surfaces of a three-dimensional polyhedron, where the surfaces contain unstretched, identical tiles, on the spherical surface. Among the full list of polyhedra, those that follow the symmetries of Platonic solids, three-dimensional polyhedra with flat faces that are all the same regular polygons, are considered here, as they exhibit high space-group symmetries. These include full icosahedral (I_h), full octahedral (O_h), full tetrahedral (T_d), and N -dihedral (D_{Nh}) groups, as they contain the greatest number of symmetry operations. The corresponding polyhedra, including their truncated versions, are considered in our enumeration. Those that can be fitted with triangular and square tiles on their surfaces are identified and listed below in Sect. 3.1.1, 3.1.2, and 3.1.3.

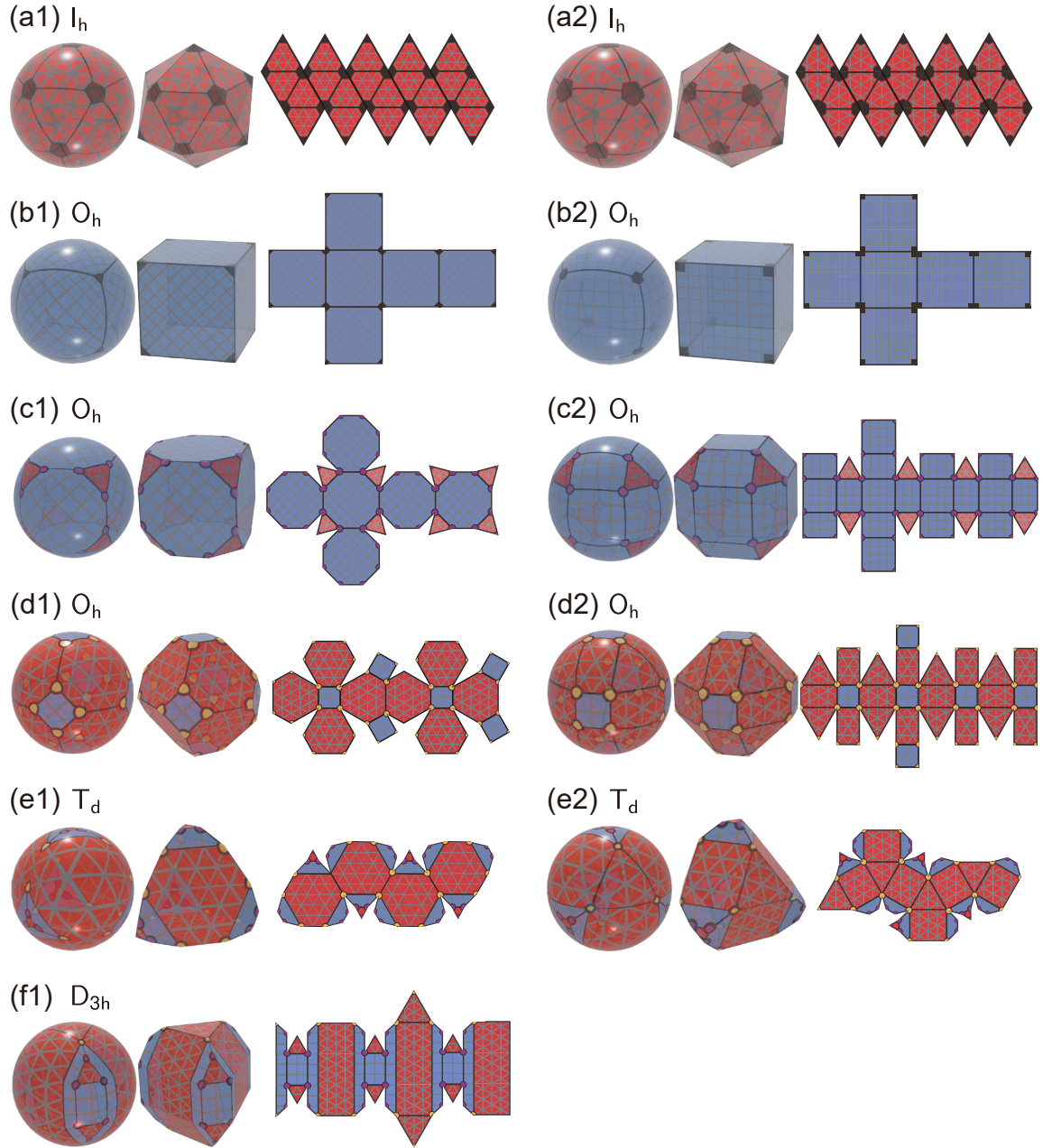


Figure 3.2: Highest symmetries of defect patterns, determined for (a1)-(a2) triangular tiling [in [3]], (b1)-(b2) square tiling [(b2) suggested in [4]], and (c)-(f) mixed tiling [found in this work.] The first panels in these plots show 3D views of the patterns on the spherical surface, and the second panels display 3D views of the projected polyhedron, which further reveal the corresponding point-group symmetry. The third panels present flattened, cut views of the second panels. All triangular-tile domains are colored red, and all square-tile domains are colored blue. The polyhedra in (c1), (d1), and (e1) are a truncated cube, truncated octahedron, and truncated tetrahedron. The polyhedra in (c2), (d2), and (e2) are cantellated cube, cantellated octahedron, and cantellated tetrahedron. The solid lines on the spherical surfaces are not necessarily geodesics; they are included solely for illustrative purposes when projecting the polyhedron onto a spherical surface.

3.1.1 Triangular tiles

The first example reviews the well-known symmetric defect patterns formed by triangular tiles. The icosahedral point-group symmetry is the highest symmetry that can be formed by twelve $w = +1/6$ defect points, located at the corner vertices of an ideal icosahedron (I_h). These vertices exhibit local five-fold symmetry around the defects and are represented in Fig. 3.2(a1) and (a2) by pentagonal defect points.

There are two different tiling patterns that accommodate low triangular lattice distortions over the entire spherical surface, icosahedron [first panel of Fig. 3.2(a1)] and dodecahedron [(a2)], each having their unique tile orientations with respect to the nearest defect-defect geodesic curves. This is more clearly observed in the polyhedron view, shown in the second panels of the plots. Along these curves, the edges of the triangles are consistently aligned to form a global structure in the icosahedron pattern. This alignment is easily understood by viewing the flattened-out icosahedron, before its projection onto the spherical surface [Fig. 3.2(a1), third panel]. In the dodecahedron pattern, on the other hand, the nearest defect-defect geodesic curves are always perpendicular to one of the edges of the triangles that fill the surface domains in between. This can again be visualized in the flattened-out view in Fig. 3.2(a2), third panel. Around the twelve $+1/6$ point defects, each pattern contains distorted triangular lattices that form twelve local pentagons, identical in shape. The relative orientations of the pentagons differ between the two patterns.

From symmetry alone, no conclusion can be drawn about which pattern, (a1) or (a2), has lower energy, since the two structures are identical from an elastic theory perspective [87]. Simulations [88, 87] were conducted to compare the elastic energies of the two symmetries shown in (a1) and (a2). The simulation revealed a slight energy difference between the two states, with (a2) having the lower energy.

3.1.2 Square tiles

The point disclination with the lowest positive winding number is $+1/4$ for square lattices [Fig. 3.1(b)]. To tile the spherical surface with only $+1/4$ defect points, eight defect points must be distributed across the spherical surface. Following the same basic principles that lead to the defect patterns discussed in the previous section, the basic defect pattern is cubic, with full octahedral O_h point-group symmetry. The defect points, which have three-fold local symmetry, are positioned at the corner vertices of a perfect cube [Fig. 3.2(b1) and (b2)].

Depending on the orientations of the square tiles, there are two different defect patterns that result in the least lattice distortion: (b1) and (b2), both possessing the global full

octahedral group O_h .

The first cubic pattern is shown in Fig. 3.2(b1). Near the point-point line connecting two nearest defect points, the square tiles are diagonally arranged such that the two diagonal vertices align with the point-point line [see the polyhedron view in Fig. 3.2(b1)]. The second cubic pattern is shown in Fig. 3.2(b2). Near the line connecting the two nearest defect points, the edges of the square tiles are aligned parallel to the defect-defect line [see the polyhedron view in Fig. 3.2(b2)]. The difference between the two patterns can be easily identified in the flattened, cutout views in Fig. 3.2(b1) and (b2). Each of these two patterns has eight identical local defect regions, forming triangular defect domains.

3.1.3 Mixed triangular and square tiles

The main subject of this study is the mixed triangular-square tiling. Since the lowest possible positive defect point has a winding number of $+1/12$, twenty-four defect points are distributed over the spherical surface. In this case, there are four possible high-symmetry defect classes. All illustrations here contain triangles and squares of the same side lengths. When they have different side lengths, the lattice boundaries between the triangular and square domains may exhibit distortion to match the bond lengths. Here, we assume that the distortion is localized to the boundaries, for which the boundaries in the illustrations are conceptual and should be viewed as narrow corridor regions.

The first class of patterns is the natural extension of the cubic patterns from the pure-square tile case, where $f \lesssim 1$. The defect domains at the vertices of the cube already have a triangular shape [Fig. 3.2(b1) and (b2)]. Two defect patterns are possible, following the O_h point group.

With triangular tiles added, the pattern in Fig. 3.2(c1) is a truncated cube, where the triangular tiles fill the truncated triangular areas and the square tiles fill the cubic surface, with the square edges rotated by $\pi/4$ from the cube edges [see the first and second panels of Fig. 3.2(c1)]. The diamond pattern appears on the main cube faces.

The other pattern is a cantellated cube, shown in Fig. 3.2(c2). The cantellation operation can be understood as truncating the vertices of a regular polyhedron while simultaneously chamfering the edges, creating new faces at edges and vertices. The eight triangular domains still occupy the original cube corners but are rotated so that their edges align with the direction of the cube edges. The square lattices on the main cube surfaces form a pattern that matches the original cube edges. The twenty-four defect points, shown in the plot as orange circles, are located at the corners of the triangular areas. These points

can be viewed as $w = +1/12_\Delta$ defects of the type shown in Fig. 3.1(c), corresponding to the insertion of triangles among the majority square tiles.

The second class of patterns, octahedral, also possesses O_h symmetry but is rich in triangular lattices, as shown in Figs. 3.2(d1) and (d2). When projected onto the polyhedron surfaces (second panels), these are truncated versions of originally regular octahedra. The corner-truncated version in (d1) contains six square domains at the corners of the octahedron, which are filled with square tiles. The main faces of the octahedron, shaped like triangular domains, are filled with triangular tiles. The other pattern, in (d2), is derived from (d1) by rotating all the square domains by a $\pi/4$ angle. This is best described as a cantellated octahedron, where the vertices and edges are orderly truncated. In this case, the square-domain edges are now all parallel in the cut-out view (third panels of Fig. 3.2(d2)). In both cases, (d1) and (d2), the twenty-four defect points are located at the corners of the rectangular domains. These points can be viewed as $w = +1/12_\square$ defects, as shown in Fig. 3.1(d), corresponding to the insertion of square tiles among the majority of triangular tiles.

The third class of patterns displays another major space-group symmetry, tetrahedral, T_d , shown in Figs. 3.2(e1) and (e2). The main faces of the original tetrahedron have a natural triangular shape (second panels), which accommodates the filling of triangular tiles. Square tiles begin to fill the truncated corners of the tetrahedron in both (e1) and (e2), which have a natural triangular domain shape. However, this arrangement is not sustainable near the domain center, where triangle domains filled by triangular tiles reoccur as insets. Two patterns of T_d are possible: truncated tetrahedron and cantellated tetrahedron, where the triangular domains at the corners of the original tetrahedron vertices have relatively different orientations, $\pi/3$ between (e1) and (e2). Because a square-tile domain only appears to enclose another triangular-tile domain, this structure can be stabilized at low f .

The fourth class is a truncated version of spherical hosohedron, shown in Fig. 3.2(f1), displaying the D_{3h} symmetry, where the three-fold rotation axis is along north-south poles. In the truncated version, second panel of Fig. 3.2(f1), the north and south poles are located at the centers of the top and bottom triangular domains, where triangular tiles can be fitted to. Three symmetric biangle regions, outlined by the blue square tile domains, start and end with a pair of $w = +1/12_\square$ defect points (hence a total of six defect points). The other eighteen defect points of the type $w = +1/12_\Delta$ appear inside the three biangle regions, and are located at the corners of two triangle domains of triangular tiles within each biangle region. This complex structure is expected to exist in the low- f range.

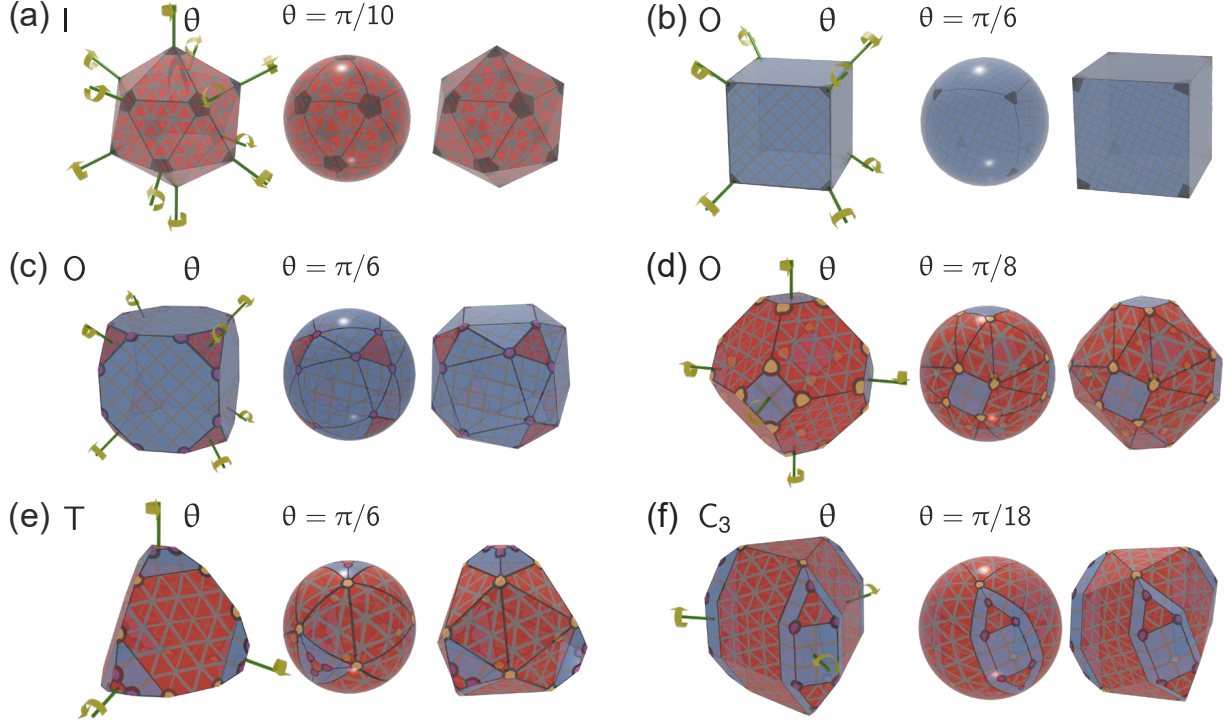


Figure 3.3: Face rotations (kaleidoscopic rotations) of the patterns listed on the left panels of 3.2(a)-(f). The rotation by an angle is performed simultaneously on the minor domains of each pattern, about axes that pass through the domain center and the spherical center. Such rotation maintains all tiling textures in the red and blue domains, relative to the domain boundaries. The rotational arrows illustrate a common counterclockwise FR angle θ . When $\theta = \pi/n$, where n represents the n -fold symmetry of the rotated domain, the patterns transform themselves into the patterns shown on the right panels of Fig. 3.2. Here, $n = 5$ for the pentagonal disclination in (a), $n = 3$ for (b), (c) and (e);, and $n = 4$ for (d). For a general θ ($\theta \neq 0$ or π/n), the full symmetry is broken, specifically disrupting the inversion and reflective symmetries, leading to I , O , O , O , T , and C_3 symmetries for panels (a)-(f), respectively. The corresponding spherical and polyhedral views of a FR pattern are shown in the second and third columns.

3.2 Face Rotation

The enumeration produces symmetric structures in Sects. 3.1.1, 3.1.2, and 3.1.3, but alternative, less-symmetric structures with related symmetries can also be generated. These alternatives are described in this and the next subsections.

Within the same class of defect patterns, e.g., Fig. 3.2(a1) and (a2), the main difference is the orientations of the defect domains. They are related to each other by simultaneous rotation of such domains, at an angle θ , counter-clockwise about the axis passing through the center of the defect and the spherical center. One can check that when the rotation occurs simultaneously, the boundaries of the bulk faces rotate to the same direction as well. Thus the shape of the bulk is preserved and the lattice grains of the bulk domains are rotated but not disturbed. The rotational process can be more explicitly seen on a spherical surface, having some resemblance to generating patterns seen in a kaleidoscope, maintaining symmetries and repetitions of the same local patterns [89].

This method generates an entire set of new defect patterns, as suggested by Goldberg in 1937 [81], and Caspar and Klug in 1962 [3], to manipulate the original pattern into skewed icosahedral patterns in Fig. 3.3(a), as alternatives that can occur in triangular tiling. In the following we refer to this type of operation as the face-rotated (FR) alternative.

The result is a set of skewed patterns, characterized by an angle θ . There are special cases. For example, when $\theta = \pi/5$ in Fig. 3.3(a), $\theta = \pi/3$ in (b) and (c), $\theta = \pi/4$ in (d), and $\theta = \pi/3$ in (e), starting from the patterns in Fig. 3.2(a1), (b1), (c1), (d1), and (e1), the original space-group symmetries are recovered. The defect patterns are rotated to those in Fig. 3.2(a2), (b2), (c2), (d2), and (e2), exactly. However, at an arbitrary FR angle θ between $\theta = 0$ and the specific values mentioned above, the system loses the highest symmetry of the original pattern; typically the inversion symmetry is destroyed. In our case, the kaleidoscope patterns in Fig 3.3(a), (b), (c), (d), (e), and (f) have point-group symmetry I , O , O , O , T , and C_3 respectively, which can be compared with the original I_h , O_h , O_h , O_h , T_d , and D_{3h} in Fig. 3.2.

The FR operation for the hosohedral structure is limited due to the curved boundaries of the large truncated faces, as shown in Fig. 3.2(f1). When θ is small, adjacent lattice domains can still undergo rotation. However, at larger values of θ , such as $\theta = \pi/2$, three domains lie horizontally along a great circle. This configuration makes it impossible to tile the entire surface with a single triangular lattice, as the curvature prevents seamless tiling of the bulk area.

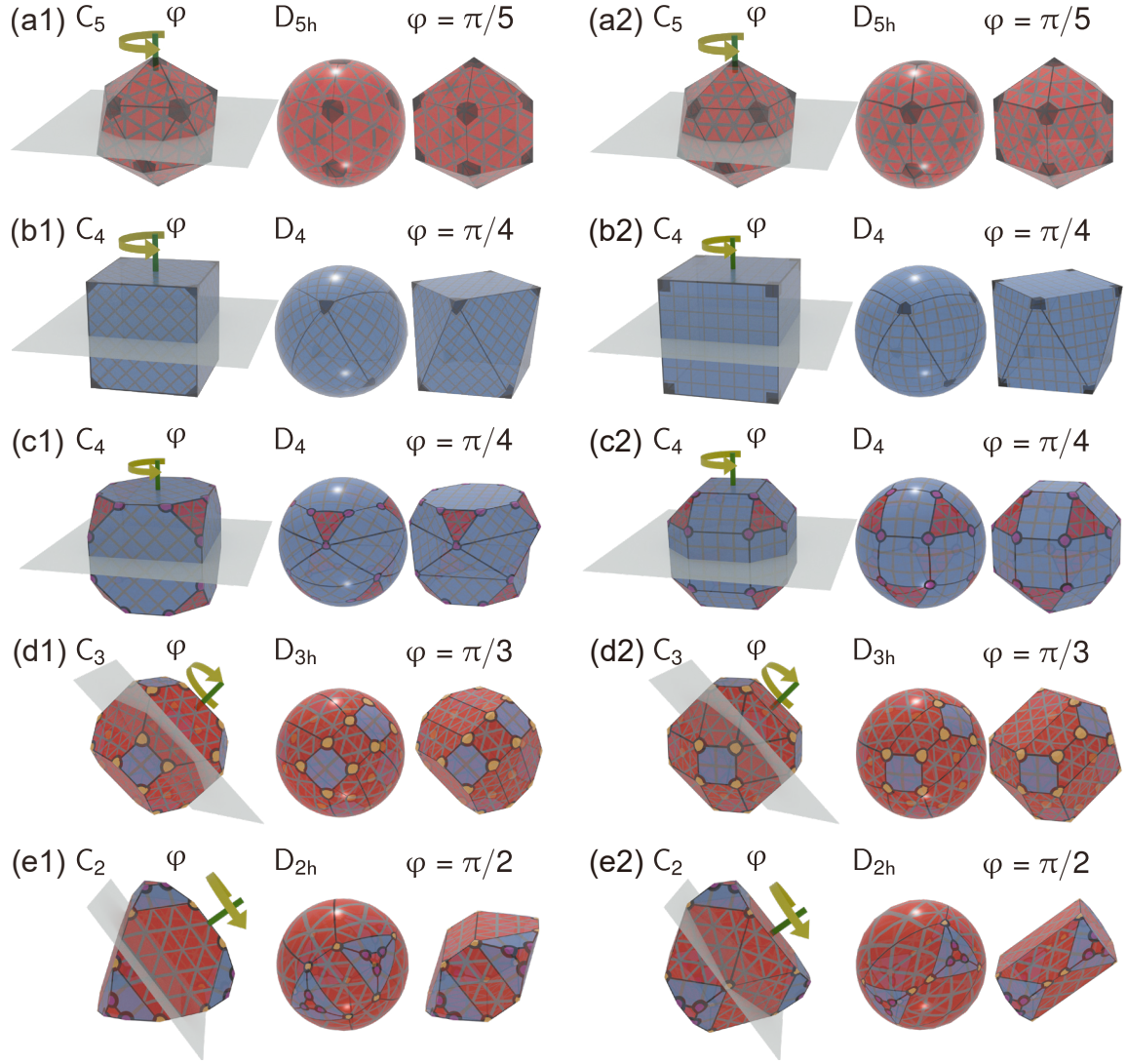


Figure 3.4: Cut-and-rotate operations on the defect patterns listed previously. The translucent plane represents the equator plane where the polyhedron is cut into two half. When projected onto a sphere, the lattice grain details at the cutting seam are identical after the CR operation. The angle φ describes counterclockwise rotation of the upper hemisphere about the spherical axis. For an arbitrary φ , the patterns in the first columns of the illustrations have space-group symmetries C_5 , C_4 , C_4 , C_3 , and C_2 for panels (a)-(e), respectively. When $\varphi = \pi/n$, where n corresponds to the n -fold symmetry of a hemisphere along the axis: $n = 5$ for (a), [i.e., $n = 4$ for (b) and (c), $n = 3$ for (d), and $n = 2$ for (e)], a higher symmetry is achieved. Specifically, the structures in the second (3D view) and third (polyhedral view) columns of the illustrations have space groups D_{5h} , D_4 , D_4 , D_{3h} , and D_{2h} for (a)-(e), respectively.

3.3 Cut-and-rotate patterns

The phrase cut-and-rotate (CR) was originally used to suggest a symmetry operation in a nematic liquid on spherical surface [37, 86]. The two +1 hedgehog point defects at the two opposite poles are cut by a great circle through the center, creating four +1/2 split defects. The entire pattern is then rotated by an angle about the common axis of the two hemispheres. In crystalline solids, a similar operation to generate related crystal structure, the mono-twinned operation, cuts along a plane followed by a rotational symmetry about the common axis [90].

Here, we borrow the same concept to create new defect patterns for the spherical lattice system currently studied. As it turns out, CR states may have a lower energy than the original patterns, as discussed in the next section. The CR operation takes an existing rotational-symmetry axis of structures in Fig. 3.4 and cuts through the equatorial plane perpendicular to the axis provided that such a cut does not split an existing defect point. The upper hemisphere of the pattern is rotated by an angle φ counter-clockwise about the rotational axis. A useful feature to consider is that, after the CR operation, the same gear-tooth-like configurations are recoverable, exactly matching the fine lattice grains on the two hemispheres at special values of φ . In theory, φ can only adopt discrete values to match this requirement; at the continuum limit, on the other hand, the lattices on both hemispheres along the cutting seam have the same fine configurations, and the rotation is smooth and continuous.

Given that the lattices here are made of triangular and square tiles, we discover that the CR operation can be performed on full symmetric patterns in Fig. 3.2(a)-(e) and most of their FR counterparts in Fig. 3.3(a)-(e) discussed above. The CR operations are illustrated in the first column of Fig. 3.4 together with the cutting planes. At an arbitrary CR angle φ , such a rotation destroys mirror symmetries of the original configuration, thereby producing a lower symmetry alternative. For example, the operations in panels (a)-(e) yield symmetries C_5 , C_4 , C_4 , C_3 and C_2 respectively, in comparison with the original I_h , O_h , O_h , O_h and T_d in Fig. 3.2. The hosohedral structure in Fig. 3.2(f1) does not have a valid cutting seam to conduct the CR operation.

There are special cases. When the angle $\varphi = \pi/n$ is used on a CR operation about a n -fold axis of the original patterns, a new symmetric pattern can be produced. The patterns shown in the second (3D view) and third (polyhedron view) columns of Fig. 3.4(a)-(e) have the point-group symmetries D_{5h} , D_4 , D_4 , D_{3h} and D_{2h} respectively. Essentially, in comparison with those with an arbitrary φ , an original mirror symmetry is recovered, which results in the higher symmetries. In comparison with the original full symmetries, some of the rotational symmetries operations are removed, hence the second and third

columns of Fig. 3.4 have lower symmetries. Considering the phrase anti-cube is already used for the special case of a CR cube, shown in Fig. 3.4(b), the names anti-icosahedron [for (a1)], anti-dodecahedron [for (a2)], anti-truncated cube [for (c1)], anti-cantellated cube [for (c2)], anti-truncated octahedron [for (d1)], anti-cantellated octahedron [for (d2)], anti-truncated tetrahedron [for (e1)], and anti-cantellated tetrahedron [for (e2)], are given for the corresponding special structures.

As a final note, triangular tiling on a spherical surface has been extensively discussed in the literature. However, the CR version of the structures, in particular, anti-icosahedron and anti-dodecahedron, have not been commonly realized as possible alternatives to the original defect patterns. One example is the stable D_{5h} structure observed in C_{70} Fullerene [13], which possesses twelve pentagons at the vertices of a pentaprism. Theoretically, it can be visualized as the CR of an angle $\varphi = \pi/5$ from icosahedral symmetry of a C_{60} Fullerene, though ten additional particles need to be inserted in the equatorial plane.

3.4 Summary

In this chapter, we have listed all possible high-symmetry tiling patterns for triangular, square, and mixed triangular-square lattices on spherical surfaces. Only low winding number point disclinations are considered in the symmetry analysis. Variations of the symmetric patterns, allowing face rotations of the defect regions and cut-and-rotate operations through an equatorial plane, are also introduced, which may lower the global defect symmetries. In Table. 3.1, we compare our constructions with structures found in previous research.

These constructions provide a pathway for comprehensive classification of possible defect structures, and serve as useful initial configurations for numerical simulations and theoretical models of self-assembly on curved surfaces. Moreover, they may inform the design of synthetic colloidal shells, virus capsids, or patterned spherical membranes where geometric frustration plays a key role in determining structural stability and mechanical response.

Table 3.1: Comparison of previous research results on various systems and their symmetries with our spherical mixed tilings.

First author	System	Symmetries found	Corresponding figures of ours	Figures of ours
Caspar[3]	Triangular lattices	I_h, I	Fig. 3.2(a1), (a2); Fig. 3.3(a)	
Altschuler[88]	Thomson problem	I_h, I	Fig. 3.2(a1), (a2); Fig. 3.3(a)	
Bowick[91]	Thomson problem	I_h	Fig. 3.2(a1), (a2)	
Li[25]	Tetratic liquid-crystals	O_h, D_4	Fig. 3.2(b2); Fig. 3.4(b2)	
Manyuhina[4]	Tetratic liquid-crystals	O_h, D_4	Fig. 3.2(b2); Fig. 3.4(b2)	
Lai[82]	Protein blocks	O_h, C_{3h}, T_d	Fig. 3.2(d),(e); Fig. 3.3(e)	
King [84]	Protein blocks	T_d	Fig. 3.2(d)	
Kroto[13]	C60 and C70 Fullerene	$I_h; D_{5h}$	Fig. 3.2(a); Fig. 3.4(a)	
Chen[83, 92]	Cone-shaped particles	I_h, O_h, T_d	Fig. 3.2(a), (b), (d), (e)	
Bowick[93]	Triatic liquid-crystal	O_h	Fig. 3.2(d)	
Echieverria[20]	Spherical lattices	I_h, I, O_h	Fig. 3.2(a),(b), Fig. 3.3(a)	
Teo[94]	triangular-square lattice	O_h	Fig. 3.2(d1)	

Chapter 4

Elastic Energy

In the previous chapter, we introduced a construction method for mixed triangular and square tiles on spherical surfaces. While physicists are often inclined to compare the energies of different configurations, such a comparison can be challenging without microscopic details such as particle interactions and densities. In this chapter, we adopt a coarse-grained model to analyze the energetic preferences among the symmetries discovered from tiling methods.

There are several levels of theoretical approaches that can be taken to study the defect patterns arising in a physical problem on a curved surface. At the molecular level, computer simulations can be performed based on a chosen molecule-molecule interaction [36, 95, 37, 50, 96, 97]. Typically, a large number of molecules are placed in the system, which yields a final global pattern of the molecular positioning and orientation (if the molecules are anisotropically shaped). At a coarse-grained, field-based model, a vector or scalar density field, typically depending on the locations on the spherical surface, is designated as the order parameter; the system's energy is expressed in terms of the field and then minimized. Examples include the phenomenological descriptions of liquid-crystal patterns based on the Landau-de Gennes theory [98, 99, 100, 101], Onsager model [102, 103, 104], Lebwohl-Lasher model [105, 95], Rapini-Papoular model [106, 107] as well as Oseen-Frank model [108, 23, 109, 110, 25, 111].

There is an even higher coarse-grained level, which emphasizes the stress on the distorted patterns on a curved surface, in comparison with their flat-space regular patterns, in the form of defect-defect interactions. At this level, the system energy is approximated by the interactions of isolated defect points, mediated by the microscopic molecular composition and surface density variation, which are not explicitly considered. In the ocean of background lattices formed by the actual molecules, the BNT potential energy, developed

by Bowick, Nelson, and Travesset, provides a simple expression for the free energy that only depends on the types and positions of the defects [21, 87]. In liquid-crystal theory, such an approach is also possible [24].

We adopt the Bowick–Nelson–Travesset (BNT) interaction as a general framework for describing the global elastic energy of disclination patterns. For an isotropic elastic sheet on a flat surface, the deformation induced by point disclinations is governed by the Airy stress potential $\Phi(\mathbf{r})$, which satisfies the inhomogeneous biharmonic equation

$$\nabla^4 \Phi(\mathbf{r}) = \sum_i w_i \delta(\mathbf{r} - \mathbf{r}_i), \quad (4.1)$$

where w_i is the winding number of the i -th disclination located at $\mathbf{r}_i$. Once appropriate boundary conditions are imposed, Φ can be solved analytically or numerically, and the total elastic energy is then computed from the corresponding energy functions.

BNT extended this flat-space formalism to curved geometries, notably the sphere, by replacing the planar Green’s function with its spherical counterpart. The resulting BNT elastic energy is given by

$$\Delta E = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n K_{ij} \chi(\beta_{ij}) + \sum_{j=1}^n \epsilon(w_j), \quad (4.2)$$

where n is the quantity of disclinations; w_i is the winding number of the i -th disclination; K_{ij} is the reduced stretching modulus between defect points i and j and $\epsilon(w_j)$ is the core energy of an isolated defect. In our notation, a $w_i w_j$ factor in the first term has been absorbed into the reduced K_{ij} . The interaction energy is written in terms of the geodesic angle β_{ij} between the i -th and j -th defect points, such that

$$\chi(\beta) = 1 + \int_0^{(1-\cos\beta)/2} dz \frac{\ln(z)}{1-z} \quad (4.3)$$

One can show that the interaction function $\chi(\beta)$ is repulsive [see Fig. 4.1].

4.1 Energy curves

For the current problem, there are $N = 24$ defects of types $w = +1/12_\square$ or $w = +1/12_\triangle$. For simplicity, in this section, a one- K approximation, $K_{ij} = K$ is taken, and the last sum is dropped, assuming two types of $+1/12$ defects have the same effects. In all cases

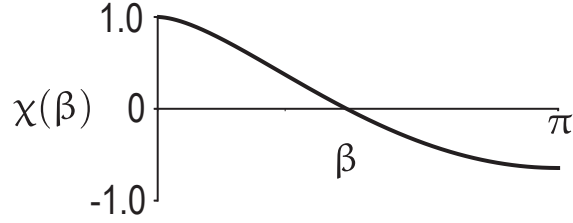


Figure 4.1: The BNT interaction energy, $\chi(\beta)$ in Eq. 4.3 between two defect points, is displayed as a function of the geodesic angle β between them.

considered below, an area fraction f is used to represent the area fraction of the square lattice regions on the curved surface, composed of geodesic boundaries.

For each class, the total BNT energy is calculated according to (4.2) with fixed values of square tiling area fraction f , CR angle (Sect. 3.3) θ , and FR angle (Sect. 3.2) ϕ , when all geometric features are fixed. Fig. 4.2(g) summarizes our findings for a given f , showing the different symmetry branches: cubic (blue), tetrahedral (orange), octahedral (green), and hoshedral (red). Vertical dashed lines mark the boundaries where the energy minimum transitions from one branch to another.

As the first example for small f within $f = [0, 0.13]$, the energy minimum ΔE^* of the tetrahedral pattern is located at $\varphi = 0$ and a nontrivial value of θ , shown in Fig. 4.2(a). The FR pattern T is the most stable. This can be physically understood by the illustration in the left panel in Fig. 4.2(a). For small- f , the square lattices only occupy the narrow edges of the truncated domains; however, the affected defect domains can be significantly large. The large square lattice domains (blue color) require the rotation of the defect regions, to avoid the direct collision of the blue regions. The calculated ΔE^* is displayed in Fig. 4.2(g), where region (a) highlights the stability of T .

As f increases further, within $f = [0.13, 0.34]$, the octahedral patterns have a lower BNT energy than T , taking over the energy branch of the T pattern. The energy plot in Fig. 4.2(b) shows that the octahedron O_h pattern in Fig. 3.2(d2) has the energy minimum in $f = [0.13, 0.24]$, where $\theta = \pi/4$ and $\varphi = 0$. In the relatively larger $f = [0.24, 0.34]$ region, the blue square domains in Fig. 4.2(c) begin to interact more significantly and the face-rotated version, O shown on the left panel of Fig. 4.2(c), has a lower energy minimum. These two regions, (b) and (c), are represented in Fig. 4.2(g) by the light and dark green shades.

In the middle f region, $f = [0.34, 0.44]$, the FR cubic pattern, which has the symmetry

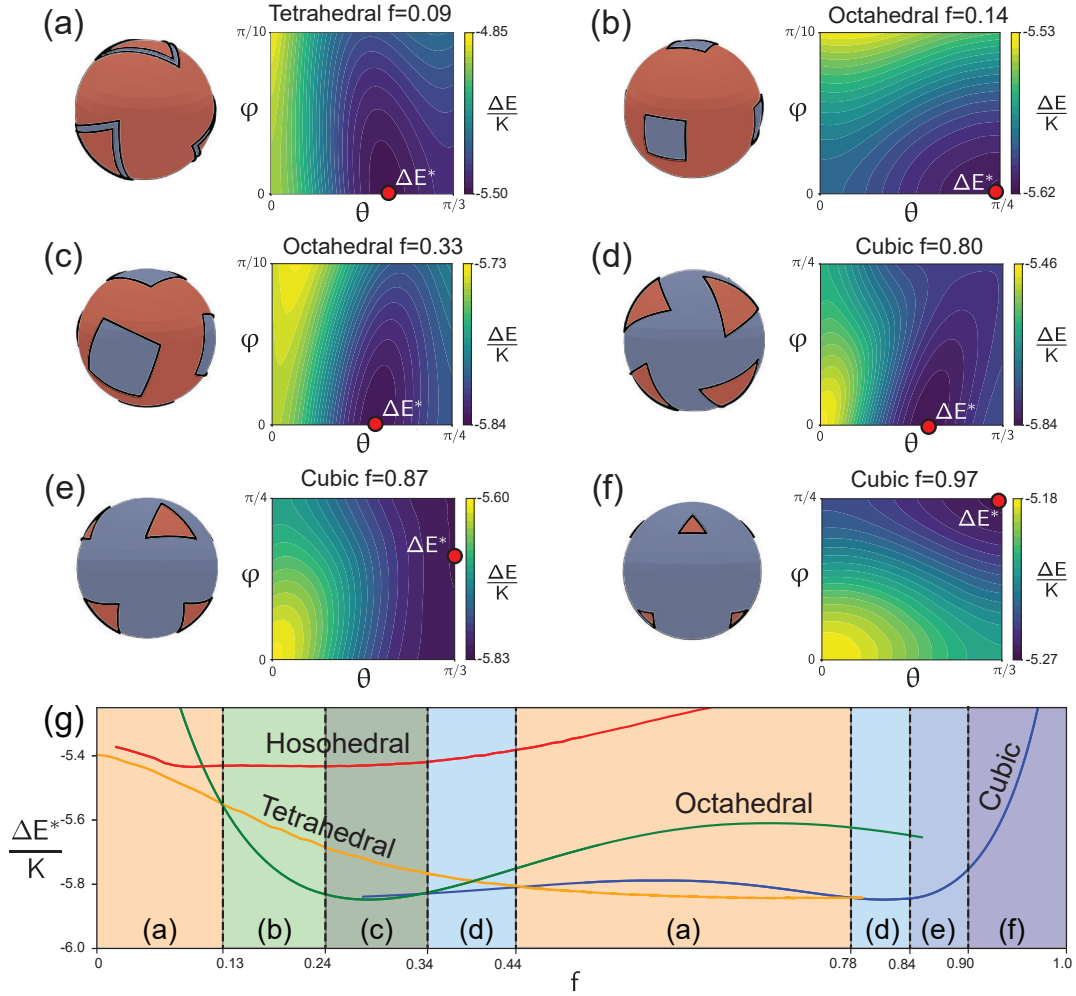


Figure 4.2: BNT energy of all studied defect patterns for a given f . Typical defect domains that exhibit the lowest BNT energy minima are illustrated below. (a) Tetrahedral pattern at $f = 0.09$, ΔE^* at $(\theta, \phi) = (2\pi/9, 0)$. (b) Octahedral pattern at $f = 0.14$, ΔE^* at $(\pi/4, 0)$. (c) Octahedral pattern at $f = 0.33$, ΔE^* at $(3\pi/16, 0)$. (d) Cubic pattern at $f = 0.80$, ΔE^* at $(2\pi/9, 0)$. (e) Cubic pattern at $f = 0.87$, ΔE^* at $(\pi/3, \pi/6)$. and (f) Cubic configuration at $f = 0.97$, ΔE^* at $(\pi/3, \pi/4)$. In each plot, the energy surface $\Delta E(\theta, \phi)$, as a function of the FR angle θ (See Sect. 3.2) and CR angle ϕ (see Sect. 3.3), is also displayed, where the location of the energy minimum is indicated by a red circle. Plot (g) summarizes our findings for a given f , showing the different symmetry branches: cubic (blue), tetrahedral (orange), octahedral (green), and hosohedral (red). Vertical dashed lines mark the boundaries where the energy minimum transitions from one branch to another.

O , has a lower energy minimum. The energy plot is shown in Fig. 4.2(d), indicating a non-trivial θ value, an FR alternative of Fig. 3.2(c2). In this middle- f region, the defect points are evenly spread out on the spherical surface. The configurational differences of the spreading, of the tetrahedral pattern in (a), the octahedral pattern in (c) and cubic in (d), give rise to minor energy-minimum differences, where the three branches of the energy curves in (g) are closely spaced.

In the mid-high region, $f = [0.44, 0.78]$, the close energy difference between T pattern in (a) and O in (d) remains. The patterns in Fig. 4.2(a) re-enter as the most stable pattern. The evenness of defect spreading on the surface can also be observed in both cases.

Coming from the high- f side, $f = [0.78, 1]$, the cubic patterns are most stable. Near $f = 1$, the pattern corresponding to a lower space-group symmetry D_4 has a lower energy, where $\theta = \pi/3$ and $\phi = \pi/4$. The pattern is a CR alternative of the pattern in Fig. 3.2(c2), i.e., Fig. 3.4(c2). The energy plot on the right panel of Fig. 3.2(f) indicates that the patterns in Fig. 3.2(c1) and (c2) are not even meta-stable; one is actually an energy maximum and the other saddle point.

Across $f = 0.90$ from the high- f region, the perfect CR alternative loses its D_4 symmetry, as φ is lowered from the ideal $\pi/4$ value. A general CR alternative is observed. As $f = 0.84$ is approached from the high- f side, φ starts to approach another ideal value, $\varphi = 0$. The cubic pattern in Fig. 3.2(c2) is realized at a single value of $f = 0.84$, where its saddle-point energy becomes a true minimum.

Below $f = 0.84$, an FR alternative of the pattern illustrated in Fig. 4.2(e) appears as the energy minimum. Starting from the ideal pattern, the defect regions in Fig. 3.2(c2), begin to face-rotate, towards the pattern in Fig. 3.2(c1) as the would-be target. The cubic energy minimum branch is the lowest among other possibilities in the region $f = [0.78, 0.84]$.

Figure 4.2(g) presents all BNT energies of the patterns described above. A few remarks can be made about the general features. (a) The hosohedral pattern indeed shows an energy minimum at $\theta \approx \pi/18$ and $f = 0.09$, but that branch, represented by the red curve in the plot, is always higher than the others. Thus, the hosohedral patterns are only meta-stable. (b) All energy minimum curves correspond to either an FR or CR alternative, but never both. There is only one energy minimum on the two-dimensional $\Delta E(\theta, \varphi)$ plots, hence only a single stable (or meta-stable) pattern for a given f within a given class of patterns. (c) The results have been presented as a function of simultaneous face-rotation of all defect regions of a given ideal pattern, at a common angle θ . We have also tested another possibility, namely, allowing all defect regions to rotate independently from each other using a minimization calculation. The process all converges back to the same θ rotation. Thus, the physical picture of simultaneous face-rotation is justified. (d) The

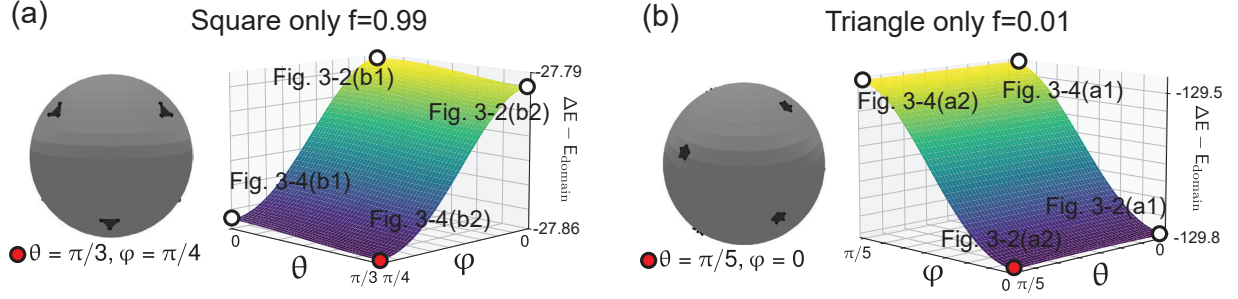


Figure 4.3: Limit-approximation BNT energy for the square and triangular pure-tiling limits. (a) Pure-square case ($f = 0.99$). The energy landscape shows the elastic energy $\Delta E - E_{\text{domain}}$ for a cubic (O_h) configuration as a function of FR and CR angles, (θ, ϕ) respectively. The red dot marks the energy minimum, which corresponds to the configuration shown on the left sphere, and to the tiles shown in Fig. 3.4(b2). (b) Pure-triangle case ($f = 0.01$). The energy surface is calculated for an icosahedral (I_h) configuration, as a function of (θ, ϕ) . Here, f denotes the fractional area of pentagons that represents a $+1/6$ disclination. The energy minimum (red dot) corresponds to the configuration shown on the left, and to the tiles shown in Fig. 3.2(a2)

systems with larger square domains tend to form the FR patterns. To avoid the closing of repulsive defect points, a rotated pattern spreads out the distance between the defects more evenly.

4.2 Pure square tiles

We now return to the case of tiling the spherical surface by square tiles only, the possible defect symmetries are cubic the CR/FR alternatives presented in Chapter 3 respectively. In this section, we use a limiting approximation method to approach the pure square-tiling limit ($f \rightarrow 1$) from mixed Hex-Sq lattices. This approach allows us to compare energy differences between different square tiled symmetry patterns using the one- K approximation of the BNT elastic energy model.

In the limit $f \rightarrow 1$ for the cubic symmetry classes that are mainly square tiled, three $w = +1/12$ disclinations, located at the corners of a triangular shaped domain [see Fig. 4.2(d-f)], merge into a single $w = +1/4$ defect. The shrinking triangular domains retain the necessary square-grain texture near these defects, enabling an effective mapping onto the pure square-tiling problem. Under this approximation, the BNT energy for the square-only

configuration can be estimated as:

$$\Delta E(\theta, \varphi)|_{\text{Square only}} = \Delta E(\theta, \varphi)|_{\text{Mixed cubic } (f \rightarrow 1)} - 8E_{\text{domain}}, \quad (4.4)$$

where $E_{\text{domain}} \approx 3\chi(0)$ accounts for the internal interaction energy of the three $w = +1/12$ disclinations within each triangular domain. The term $-8E_{\text{domain}}$ reflects the removal of these intra-domain contributions.

By choosing $f = 0.99$, we approximate $\Delta E(\theta, \varphi)$ in the $f \rightarrow 1$ limit. As shown in Fig. 4.3(a), the resulting energy landscape closely resembles that in Fig. 4.2(g). According to the BNT interaction potential, a single global energy minimum emerges at $\theta = \pi/3$ and $\varphi = \pi/4$, corresponding to the anti-cubic configuration shown in Fig. 3.4(b2). The cubic configuration [Fig. 3.2(b1)] corresponds to an energy maximum, while other configurations [e.g., Fig. 3.2(b2), Fig. 3.4(b1)] lie at saddle points and are therefore energetically unstable.

These findings confirm that, in the limit $f \rightarrow 1$, anti-cubic symmetry emerges as the elastic ground state, consistent with previous results by Lubensky [23], Li [25] and Manyuhina’s “nematic like” model [4]. However, this result is not definitive. The key idea behind the limiting approximation is to introduce a small degree of anisotropy by retaining minimally sized triangular regions around each disclination. When f is very close to 1, the triangular regions are small, and the disclinations behave isotropically—favoring anti-cubic symmetry. As f decreases (i.e., larger triangular regions), meaning the anisotropy increases, and cubic symmetry may become more favorable, as shown in Fig. 4.2(d) regime. This trend is consistent with the work of Manyuhina and Bowick [4], who found that isotropic, nematic-like systems prefer anti-cubic arrangements, whereas anisotropic tetratic systems favor cubic symmetry.

Therefore, by treating the triangular domain area as a tunable parameter, this method provides a unified framework for characterizing a range of square-ordered spherical systems—from nearly isotropic ($f \rightarrow 1$) to strongly anisotropic ($f \lesssim 0.84$).

4.3 Pure triangular tiles

Finally, we return to the case of triangular tiling, the original Caspar-Klug (CK) problem. The possible global symmetries were thoroughly explored by Caspar and Klug [3], as well as Goldberg [81]. These symmetries include the icosahedral [Fig. 3.2(a1)], dodecahedral [Fig. 3.2(a2)], and skewed classes [Fig. 3.3(a)] in the context of CK constructions. For the particle number

$$N = 10(m^2 + n^2 + mn) + 2 \quad (4.5)$$

where m and n are positive integers and $m \geq n$, an icosahedral symmetry with twelve pentagonal disclinations at the vertices can be realized. From a lattice direction perspective, $(n, 0)$ corresponds to the icosahedral arrangement [Fig. 3.2(a1)], (n, n) to the dodecahedral [Fig. 3.2(a2)], and (n, m) to the face-rotated classes [Fig. 3.3(a)]. Systems with particle numbers N that satisfy Eq. 4.5 exhibit icosahedral symmetry as a low-energy state [88, 87]. Specifically, for $N \lesssim 400$, the system tends to favor the icosahedral symmetry as the ground state, while for $N \gtrsim 400$, it may become metastable due to the presence of scars.

There has been significant research aimed at investigating the differences between these symmetry classes. By direct energy minimization, Bowick et al. [87] compared the energy differences in a generalized Thomson problem between $(n, 0)$ and (n, n) systems for $N \lesssim 1000$. It was shown that the energy densities of both $(n, 0)$ and (n, n) configurations are positively linear with $1/N$. In the limit of $1/N \rightarrow 0$ (the continuous limit), the (n, n) structures exhibit lower energy than the $(n, 0)$ structures. A similar comparison was conducted by Pérez-Garrido et al. [112], where the $(23, 23)$ system with $N = 15872$ and the $(40, 0)$ system with $N = 15282$, both having similar defect configurations, were compared. It was found that the $(23, 23)$ system had lower energy than the $(40, 0)$ system. Additionally, Altschuler et al. [88] compared the energies of the skewed class (m, n) configurations with equal particle numbers, such as $(6, 5)$ and $(9, 1)$, both with $N = 912$. They concluded that systems with a smaller m/n ratio tend to have lower energy, implying that the (n, n) structure represents the ground state, while the $(n, 0)$ configuration corresponds to the maximum energy state. However, these studies are primarily based on numerical simulations that rely on specific inter-particle potentials. From a theoretical standpoint, within the framework of continuum elastic theory, the energetic distinctions between the icosahedral, dodecahedral, and face-rotated classes vanish. This is because the elastic energy in the leading-order approximation depends solely on the positions and topological charges of the disclinations, whereas the detailed internal lattice texture within each domain enters through higher-order gradient terms, which are typically neglected in standard continuum elastic theories.

Moreover, while the energy differences associated with various orientational textures have attracted considerable attention, one critical aspect has been largely overlooked: the variation in the arrangement of defect points themselves. Unlike the extended discussion for square-tiled systems, where the cubic and anti-cubic symmetries are examined carefully, the analogous transformations in triangular-tiled systems remain underexplored. Specifically, the cut-and-rotate operation in triangular tiled systems, illustrated in Fig. 3.4(a1) and (a2), has not been considered in existing studies.

Following the success in the last section, here we propose calculating the BNT energy of pure triangular tiling using the same limit-approaching trick. The original problem

in Fig. 3.2(a1), (a2), and Fig. 3.4(a1), (a2) is transformed into the task of adding twelve pentagonal defect domains. Each of these domains is composed of five imaginary defect points, each with a defect strength of $w = +1/30$, located at the vertices. The boundaries of the pentagonal defect domains preserve the grain texture of the triangular tiling as shown in Fig. 3.2(a1), (a2), and Fig. 3.4(a1), (a2). This preservation of texture is the key feature that distinguishes (a1) from (a2).

An energy similar to (4.4) is used

$$E(\theta, \varphi) \Big|_{\text{Triangles only}} = \Delta E(\theta, \varphi) \Big|_{\text{Mixed icosahedral } (f \rightarrow 0)} - 12E_{\text{domain}} \quad (4.6)$$

where f is defined as the area fraction of the gray-shaded pentagons, as shown in Fig. 4.3(b). $E_{\text{domain}} \approx 10\chi(0)$, (5 particles, considering two direct neighbors and two spaced neighbors, making $5 * (2 + 2)/2$), the internal energies of the domain are excluded as well.

At $f = 0.01$, the energy landscape for icosahedral-class configurations is shown in Fig. 4.3(b). According to the BNT model, a single global energy minimum appears at $\theta = \pi/5$, $\varphi = 0$, corresponding to the structure depicted in Fig. 3.2(a2), or equivalently, the (n, n) dodecahedral configuration in the Caspar–Klug (CK) framework. In contrast, the structure shown in Fig. 3.2(a1), representing the $(n, 0)$ icosahedron, corresponds to a saddle point with higher energy than the (n, n) configuration, in qualitative agreement with simulation results reported by Bowick [87] and Pérez-Garrido [112]. Furthermore, along the edge defined by $\varphi = 0$, the energy decreases monotonically as θ increases from the $(n, 0)$ to the (n, n) configuration, corresponding to a monotonic decrease in the ratio m/n . This observation is consistent with the findings of Altschuler et al. [88], who showed that configurations with smaller m/n ratios exhibit lower elastic energy. In contrast, the cut-and-rotate configuration shown in Fig. 3.4(a2) corresponds to the global energy maximum, while Fig. 3.4(a1) is identified as another saddle point.

Motivated by the expectation of a possible phase transition from full icosahedral symmetry to a skewed class configuration—as illustrated in Fig. 4.2(d) to (e)—with increasing domain size, we explored the energy landscape of icosahedral structures at larger values of f . However, across all values of f examined, no such transition was observed. This result indicates that, irrespective of how large the gray-shaded region (representing triangular domain area) becomes, the (n, n) dodecahedral configuration consistently remains the elastic ground state.

In conclusion, by assigning a finite geometric shape to point disclinations through the limit-approximation method, we enable a possible comparison of the elastic energy associated with different orientational configurations.

4.4 Summary

In this chapter, we employ the BNT model to perform a coarse-grained energetic analysis of the symmetry classes emerging from mixed square–triangular tilings on spherical surfaces. This analysis is based solely on the spatial arrangement of disclination points. For a given area fraction of square tiles f , only one representative configuration within each symmetry class—original or alternative—corresponds to an energy minimum. By comparing these minima across the four symmetry classes, we identify the preferred tiling pattern for specific ranges of f .

Building on this framework, we apply a limit-approximation method to explore the elastic energy behavior in the pure square- and triangular-tiled limits. This approach yields results consistent with previous theoretical and simulation-based studies, further validating the utility of this coarse-grained method in understanding symmetry selection in spherical crystalline systems.

There are several complications that may impact the final results. (a) One such complication is the finite-size effect, which already exists in the triangular-tiling problem. In a finite system, given the area of the spherical surface, there is a relationship between the total number of tiles (the magic number) and an optimal symmetry pattern. Adding another tile is likely to alter or even destroy the entire symmetry. We essentially take a continuum limit, assuming many small tiles fill the available space and that magic numbers can be naturally established for a large system. (b) Another issue unique to tiling a surface with mixed triangular-square tiles is the line tension problem between the triangular and square lattice domains. The basic components of the system are individual, pre-made triangular and square tiles. The potential mismatch in tile side lengths requires lattice distortion along the boundaries between the triangular and square lattice domains. This can significantly affect the second part of the study, as the energy produced by line tension should be incorporated into the theory. The line tension introduces an additional parameter, calling for another dimension in the state diagram presented in Fig. 4.2, which is not considered here (c) Instead of pre-made tiles, many surface structures in real systems are self-assembled from isotropic molecules. The triangular and square lattices result from self-assembly, not from a rigid structure to begin with. The coexistence of these lattices is closely related to a first-order phase transition between triangular and square crystal orderings. In this case, f should be treated as an adjustable parameter, along with the number density of the molecules, in a complete free-energy consideration. (d) In this study, we used a one-elastic-constant approximation. The difference in elastic energies (notionally represented by the K_{ij} tensor in a coarse-grained consideration) as well as the difference in the two different types of 1/12 defects (i.e., the ϵ term in Eq. 4.2) can significantly affect

the outcome of the energy analysis. (e) The use of the BNT interaction in an isotropic form, as given by Eq. 4.3, ignores the relative orientations of the defect points and their grain texture directions in between. This is already an issue, even for triangular tiling. Remedying this effect, which involves mixed media made up of triangular and square tiles, requires further research.

These complications impact the energy landscape of the problem. While the symmetry analysis in Chapter. 3 likely remains the same, the energy analysis in this chapter could be significantly altered. We hope that the current energy study captures some essential features of mixed tilings.

Chapter 5

Conclusion

In this thesis, we have explored the interplay between crystalline order, topological defects, and curvature by investigating the structural and energetic properties of mixed triangular-square lattices confined to spherical surfaces. Combining computational simulations, geometric tiling constructions, and coarse-grained elastic theories, we reveal a rich variety of defect morphologies and symmetry classes that emerge from the competition between local lattice order and global geometric frustration.

In Chapter 2, we employed molecular dynamics simulations with Hertzian interactions to self-assemble soft particles into coexisting triangular and square lattices on spherical surfaces. The simulations uncovered a range of defect structures, including not only point disclinations and scar defects but also domain and counter-domain defects that reflect crystalline-crystalline phase separation under curvature constraints. These structures exhibit global symmetries such as octahedral, tetrahedral, and cubic, depending on the area fraction of square tiles f . The discovery of counter-domain defects—where a lattice type embeds within its own defect domain—highlights the nontrivial consequences of shape frustration unique to curved surfaces.

In Chapter 3, inspired by the simulation results and symmetry considerations, we developed a systematic geometric tiling approach to construct mixed-lattice defect configurations with high symmetry. Building on the Caspar-Klug framework, we introduced face-rotation and cut-and-rotate operations to generate new classes of lattice arrangements, extending the range of possible tilings beyond previously studied symmetric forms. These constructions unify the known Platonic and Archimedean-based tilings with novel mixed-lattice configurations.

In Chapter 4, we employed the Bowick-Nelson-Travesset (BNT) elastic energy model as a coarse-grained framework to compare the elastic energies of defect configurations across

symmetry classes. This analysis was conducted solely based on the location and topological charge of disclinations, enabling an efficient comparison of the stability of different defect morphologies. A key contribution is the introduction of a limit-approximation method, in which domain defects shrink to points, allowing us to explore the energetics of pure square and triangular tilings. This approach confirms known ground-state symmetries, such as the anti-cubic pattern for square lattices and the (n, n) dodecahedral pattern for triangular lattices, and reveals the role of anisotropy in determining symmetry selection.

Overall, this thesis provides a comprehensive framework for understanding how the coexistence of distinct lattice types and the geometry of the embedding surface shape defect morphology and symmetry in soft crystalline systems. The insights gained here not only deepen our fundamental understanding of curvature-induced frustration but also point to new design principles for self-assembled nanostructures and functional materials. Future directions may involve extending this framework to other kinds of mixed lattices in dynamic systems, multilayer lattices, or alternative geometries such as tori and ellipsoids, where new classes of defects and symmetries may emerge.

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