ROYAL SOCIETY OF CHEMISTRY

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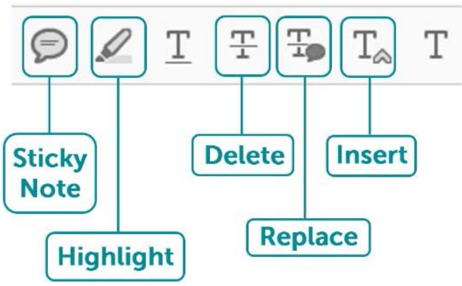

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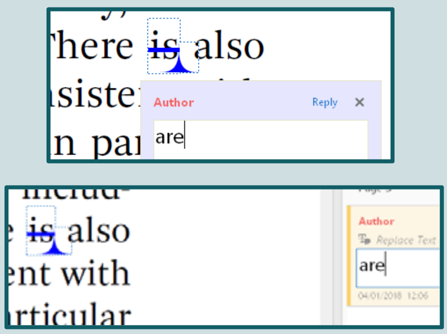

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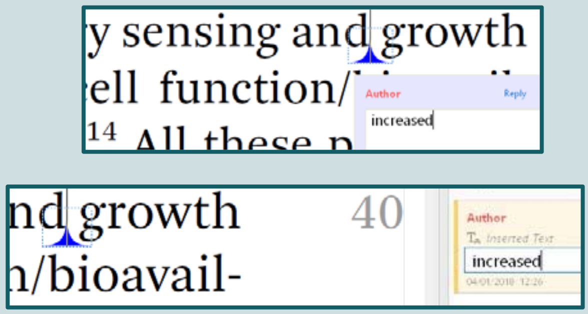

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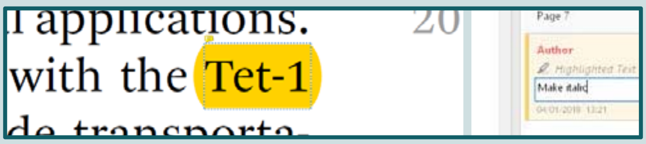

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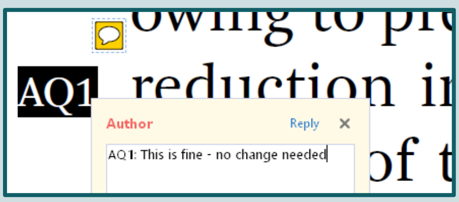

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AQ:1

Image	Short description	Long description
Figure 1.1	A photo shows a stack of large stone spheres arranged in a pyramid-like formation ~~on a grassy lawn, with a stone wall in the background~~.	
Figure 1.2	A photo and a figure, placed side-by-side, illustrate two types of tiling. On the left, the photo shows a stone tiling pattern on a bridge in Regensburg. The stones are arranged in a regular, interlocking pattern ~~that appears weathered and well-worn.~~ On the right, there is a geometric design representing a Truchet tiling, composed of square tiles, each containing a quarter-circle curve. The curves alternate in orientation across the grid, creating a continuous and flowing visual pattern of connected arcs in black and white.	
Figure 1.3	A close-up photo shows a complex network of soap films forming a dry foam with variously sized and shaped ~~interconnected~~ bubbles. The foam consists of an intricate network of thin soap films forming irregular polygonal and polyhedral shapes. The ~~compartments~~ vary in size and shape~~, with some appearing nearly hexagonal or pentagonal, while others are more distorted~~. The soap films intersect at edges ~~and vertices, creating a dense, reticulated structure.~~ The overall appearance is airy yet structured, with the fine lines of the soap films forming a visually complex, three-dimensional web.	
Figure 1.4	Figure illustrating a photo alongside a historical diagram showing stacked spheres in triangular arrangements labeled A to E.	On the left is the photo of a stone bust of Johannes Kepler, ~~positioned outdoors with leafless tree branches visible in the background.~~ The bust shows Kepler with a beard, mustache, and a high-collared garment. On the right, a black and white historical illustration shows five configurations of small, round spheres labeled A, B, C, D, and E, arranged in increasingly larger triangular patterns from top to bottom. The smallest group (A) contains a few spheres in a compact cluster, while the largest group (E) forms a broad triangular pyramid of tightly packed spheres. ~~The diagram is bordered by text written in an old-style serif font.~~
Figure 1.5	A photo shows ~~a man standing and smiling behind a pyramid-shaped stack of yellow tennis balls arranged on a table, with a chalkboard visible in the background. The man is dressed in a checkered shirt and stands~~ behind a neatly arranged pyramid of bright yellow tennis balls. ~~The balls are stacked in a triangular close-packed formation atop a wooden surface. Each tennis ball is identical, featuring red printed text.~~	
~~Figure 1.6~~	~~Figure illustrating a black and~~ white portrait of Cyril Stanley Smith on the left and a close-up photo of a two-dimensional foam structure on the right.	The portrait shows Cyril Stanley Smith with neatly combed hair, wearing wire-rimmed glasses, a collared shirt, a dark tie, and a textured suit jacket. His expression is serious and composed, and he looks directly at the camera. On the right is the grayscale photo of a two-dimensional foam structure, created by a single layer of bubbles enclosed between two transparent plates. The foam exhibits an irregular ~~yet tightly packed~~ cellular pattern with polygonal bubbles of varying shapes and sizes, ~~some forming pentagonal and hexagonal structures~~.

Image	Short description	Long description
Figure 1.7	Twelve parts labeled (a) to (l) illustrating polyhedral particles packed in different crystalline and liquid crystal structures and accompanied by shape diagrams and diffraction patterns.	Part (a) shows a dense, tan-colored cluster of small cubes stacked in a regular cubic lattice. The cube faces are labeled with crystallographic directions (100) and (010). To the right, a pair of beige polyhedral diagrams shows the individual cube shapes. A small circular diffraction pattern appears in the lower right corner, revealing sharp, periodic spots indicating a high degree of symmetry and order. The structure is labeled Cubic c P 1 (A h). Part (b) features a green-colored arrangement of elongated polyhedra arranged in a more distorted, yet periodic, pattern. Crystallographic planes (100) and (001) are marked. Diagrams of the beta-S n (tin) structure polyhedra are shown to the side, along with a red diffraction pattern. The structure is denoted as beta-S n t I 4 (A 5). Part (c) displays a teal-colored compact lattice of cube-like particles called supercubes. The particles are arranged with visible (100) and (010) planes. A red circular diffraction pattern confirms structural order. Polyhedra to the side show facets of the supercube. The structure is labeled Supercube c P 6. Part (d) shows a light tan group of irregular polyhedra forming a complex packing, surrounding a highlighted region in blue with red and green overlaid lines to indicate internal unit geometry. A detailed red diffraction image is shown beside it. The polyhedra depicted resemble irregular dodecahedra. The structure is labeled Sigma 3.4.3 squared. Part (e): A cluster of blue polyhedra in a face-centered cubic (F C C) arrangement, with crystal directions (111) and (111 bar) labeled on the cube faces. The central region features highlighted layers and an illustration of the repeating unit with truncated shapes. A bright red diffraction pattern confirms F C C symmetry. Labeled F C C c F 4 (A 1). Part (f) displays a green-colored structure in a body-centered cubic (B C C) formation. The crystal planes (100) and (010) are visible. A polyhedron with flat and angled faces is shown as a representative unit, with a red diffraction inset indicating periodic symmetry. Labeled B C C c I 2 (A 2). Part (g): An orange-brown packing of compact, irregular polyhedra representing a beta-W (beta-tungsten) structure. The central region is outlined with an orange rectangular cell. The red circular diffraction pattern indicates a high degree of symmetry. Labeled beta-W c P 8 (A 15). Part (h): Orange-colored particles arranged in a denser packing than Part (g), forming a beta-M n structure. The central region is marked with blue, green, and red lines. The diffraction pattern is more intricate than others, indicating complex symmetry. Labeled beta-M n c P 20 (A 13). Part (i) displays a rich orange structure of gamma-brass particles. A large hexagon is overlaid in the center, and the unit polyhedron resembles a truncated tetrahedron. The diffraction image shows a detailed pattern with sharp reflections. Labeled gamma-Brass c I 52. Part (j): Light pink polyhedra arranged in a loose, less ordered structure. The particles appear aligned in a common direction but lack positional order. The representative polyhedron is long and narrow. A red circular pattern with a bright center suggests orientational order. Labeled Nematic. Part (k): Dark red and cream polyhedra are arranged in horizontal layers or bands, demonstrating a smectic phase. The polyhedra are similar to Part (j) but with positional order in one direction. A bright ring diffraction pattern confirms a layered structure. Labeled Smectic. Part (l): A columnar arrangement of greenish-gray rod-shaped particles packed vertically in parallel stacks. A pentagonal polyhedron represents the packing unit. The diffraction pattern shows six-fold symmetry, indicating columnar alignment. Labeled Columnar Discotic.

Image	Short description	Long description
Figure 1.8	Three parts labeled (a) to (c) display different arrangements of colored circles packed tightly within geometric boundaries.	Part (a): 29 circles: This part shows a square-shaped boundary filled with 29 equally sized circles. The circles are packed closely together in a grid-like pattern. They are colored in varying shades of orange, yellow, and one magenta circle in the upper left corner. Most circles have small markings resembling three-way symmetry lines inside them. Part (b): 29 disks in a square: This part features a hexagonal boundary filled with 96 small, uniformly sized disks. These are tightly packed in a hexagonal grid arrangement. The disks are primarily orange and yellow, with one central magenta disk standing out. Like in Part (a), each disk includes internal markings of radial lines. Part (c): 50 disks in a circle: This part displays a circular boundary containing 50 disks of varying sizes. Each disk is numbered from 1 to 50 and has a distinct radius, with the smallest disks in magenta and the largest in orange and yellow. The disks are arranged to touch as many neighbors as possible within the circular space. Their sizes create a nested, organic pattern, with the largest disks more centrally placed and smaller ones filling gaps at the edges.
Figure 1.9	A black-and-white scanning electron microscope image shows a dense arrangement of pollen grains, each with distinct surface textures and shapes. The grains vary in size and include spherical forms covered with spiky protrusions, oval grains with patterned ridges, and smooth, round particles. Some pollen grains appear highly textured with net-like or bumpy surfaces, while others are more uniform. One large, irregularly shaped grain with three extended lobes stands out from the rest.	

Abstract

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We offer a general motivation for the several varieties of packing problems that are discussed in this volume, and introduce some of the key contributors to the long history of the subject. The rapid progress made in recent years has been driven by the development of new theoretical approaches, computer-assisted analysis of experimental samples, and extensive computer simulations.

CHAPTER 1

A Brief Overview of Packing Problems

DENIS WEAIRE,[a] ADIL MUGHAL[b] AND STEFAN HUTZLER*[a]

[a] School of Physics, Trinity College Dublin, The University of Dublin, Ireland; [b] Department of Mathematics, Aberystwyth University, Penglais, Aberystwyth, Ceredigion, SY23 3BZ, Wales, UK
*Email: stefan.hutzler@tcd.ie

1.1 Introduction

Densely packed arrangements of objects of all shapes and sizes have captured the attention of scholars for many centuries. The iconic image of stacked cannonballs (Figure 1.1 and cover of this book) has come to symbolize this fascinating field. Such packings have raised numerous mathematical questions; with the advent of the digital age, they continue to challenge our computational techniques and algorithms. Many questions remain unresolved and stimulate further exploration of this captivating subject.

As the range of packing problems has expanded, a related area of interest has emerged, focusing on the concept of tiling or tessellation (Figure 1.2). While packing involves positioning objects within a space, tiling partitions space into distinct compartments. For instance, foams (Chapter 10) can be considered as packings of deformable bubbles, which evolve into three-dimensional tilings when the liquid between the bubbles reduces to its minimum – essentially zero if the resulting soap films are regarded as possessing zero thickness (Figure 1.3). Point patterns, which might for example be made up of centres of packed spheres, can be converted to cellular structures by

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Figure 1.1 A stack of cannon balls, photographed in Rhodes, Greece, by the co-editor of this book, H.-K. Chan.

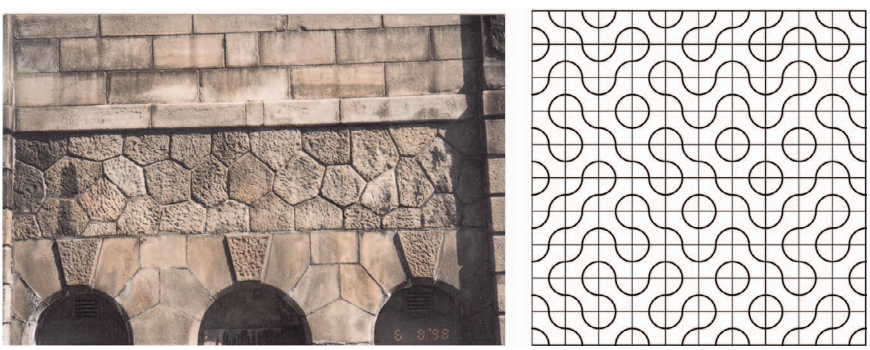


Figure 1.2 Closely related to packing problems are tilings. (left) Stone tilings at a bridge in Regensburg (Photo M. Hutzler). (right) Example of a Truchet tiling, which is a tiling made up of only one type of tile, placed in two different orientations.

the Voronoi construction.[1] There is a compelling argument for considering these two subjects as unified: often the analysis of a packing invokes a complementary tiling. Nevertheless, the present volume is focused mainly on packing.

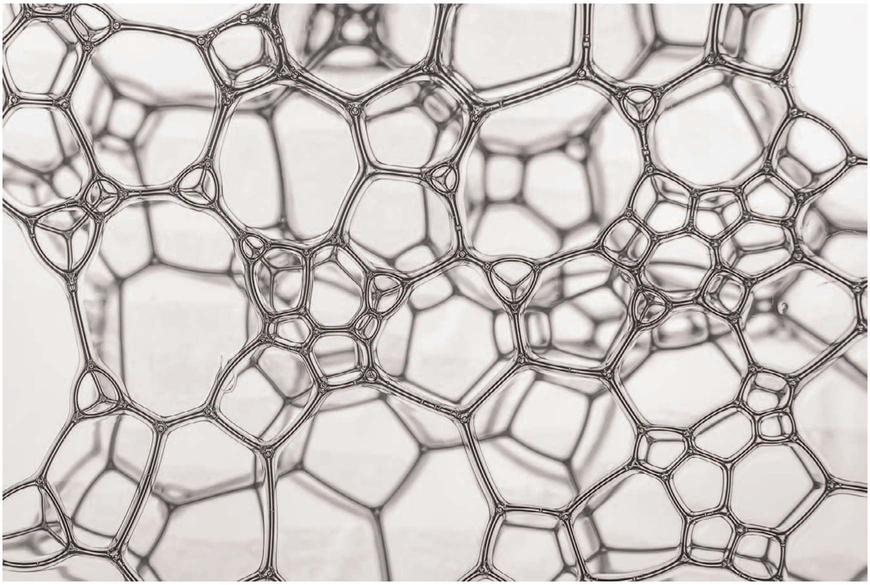


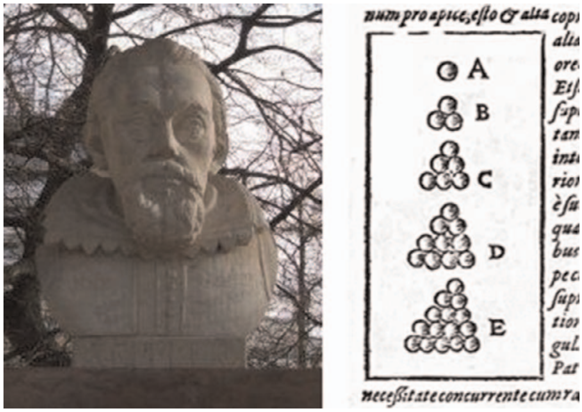
Figure 1.3 Image of a polydisperse disordered dry foam taken from the photo series “Reticulate” by art photographer Kym Cox. Courtesy of K. Cox.

1.2 Kepler’s Musings

Discussions of packing theory frequently acknowledge the early contributions of Johannes Kepler (1571–1630); see Figure 1.4. He is particularly celebrated for having formulated what has remained a long-standing question in the field, known as the Kepler Problem.[3] *What is the most efficient (densest) way to stack an infinite number of cannonballs, assuming they are perfect spheres?* Kepler hypothesized that the densest packing of spheres in three-dimensional space is achieved through a cubic close packing arrangement, as illustrated in Figure 1.1, or related stackings of close-packed layers.

Kepler formulated his ideas on sphere packing at the beginning of his 1611 booklet “A New Year’s Gift, or On the six-cornered Snowflake”.[4] They are preceded by his musings on the occurrence of hexagons in the bee’s honeycomb (a problem that was discussed already in antiquity), on space-filling structures made up of polyhedra containing only rhombic faces, and on the shape of peas that are squeezed by their pod as they grow. Interestingly, he uses the expression “materia molli” in this context (he wrote in Latin), thus predating by over 350 years the expressions “matière molle” or *soft matter* that have been in use since the 1970s to describe malleable granular materials. Kepler’s thoughts on sphere packings are just one further aside in the 1611 publication, before he finally proceeds to ponder the formation and shape of snowflakes.

The Kepler sphere-packing conjecture attracted the intellectual curiosity of numerous luminaries, including Sir Isaac Newton. However, Kepler’s



AQ:2 **Figure 1.4** Bust of Johannes Kepler (1571–1630), displayed in Regensburg, the city where he died, together with an illustration from his essay “De Nive Sexangula”.[4] ~~Courtesy of M. Hutzler.~~

Figure 1.5 Thomas Hales giving a practical demonstration of the Kepler conjecture that he proved mathematically. Photo by Bob Kalmbach, Michigan Photography, University of Michigan.

challenge – to provide a proof – stood unmet for a considerable length of time. In 1998 Thomas Hales (Figure 1.5) ventured a comprehensive conjecture that directly confronted Kepler’s age-old problem. Remarkably, his proof, especially in its initial stages, relied substantially on the method of proof by exhaustion, whereby each of a (large) set of identified individual sphere configurations is examined numerically. The final formal proof, involving Hales and 21 co-workers, and automated proof-checking software, was accepted for publication in 2017.[5]

The advent of X-ray crystallography around 1900 revealed many crystal structures, of which some could be visualised as packings. These stimulated many discussions by William and Lawrence Bragg,[6,7] and others. Their ideas (in ref. 6, for example, the crystal structure of pure bismuth is represented by the packing of spheres with three spherical caps removed) have been superseded by powerful modern theories of quantum mechanics.[8] However, studies of both ordered periodic arrangements (for example in the theory of Frank-Kasper phases of metals, or block copolymers [Chapter 20]), as well as disordered arrangements often invoke sphere packings. They also persist in that part of condensed matter theory that deals with deformable particles (Chapter 9) or "soft matter", such as foams (Chapter 10), emulsions, biological cells, granular matter (Chapters 11, 12 and 13), and colloids (Chapters 17 and 18)~~, *i.e.* systems that are usually disordered.~~

At every stage, questions have arisen for the mathematician, often simply stated (as in the case of Kepler) but elusive when pursued in search of rigorous answers.[9] Clearly, as the deplorable academic cliché goes, "the subject is still in its infancy…".

1.3 A Prototypical Soft Packing

One of us (DW) was attracted into the subject by the inspirational figure of Cyril Stanley Smith who posed interesting questions regarding the prototypical system that he adopted, the two-dimensional soap froth[10] (reprinted in 2015 as ref. 11); see Figure 1.6 and Chapter 10. He was a leading metallurgist at Los Alamos in World War II, and then gravitated to academia,

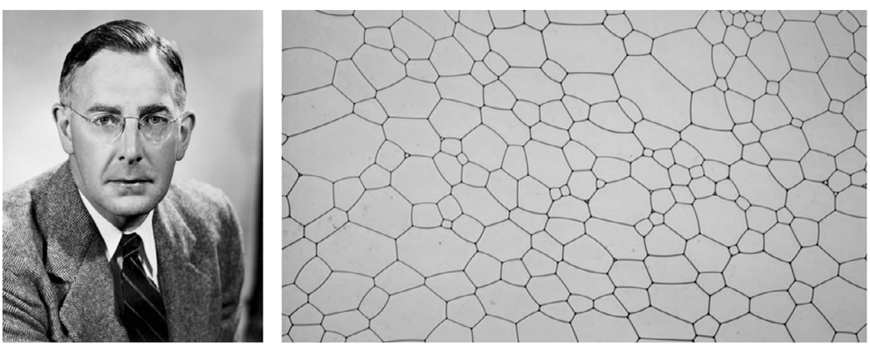


Figure 1.6 Cyril Stanley Smith (1903–1992) introduced the two-dimensional foam as a simple model system for (disordered) cellular structures. Photo reproduced from https://en.wikipedia.org/wiki/Cyril_Stanley_Smith. It is realised experimentally by sandwiching a single layer of bubbles between two glass plates; see photograph on the right. Smith was also interested in Truchet tilings,[2] such as the one shown in Figure 1.2.

founding the Institute for the Study of Metals in Chicago. Smith had a profound personal vision of materials science, decrying the exclusive pre-occupation with purely ordered structures, and called for more attention to disorder, which he identified in amorphous materials, artefacts and even art.[12]

But before Smith, many great minds were attracted to the structure of dense packings of particles, in either ordered or disordered arrangements.[13] They added to Kepler, Newton, Bragg and Kelvin. One figure that deserves special mention – the inventor of a "a simple way of looking",[14] which was just model building as opposed to mathematical analysis – is J. D. Bernal,[15] see Chapter 15. He also suggested the development of a new subject called *statistical geometry* for describing disordered packings.[16] His disordered packings of spheres have remained under investigation in recent times in the fashionable subject of "jamming",[17–19] see the discussion in Chapters 6, 8, 9 and 11, and, of relevance also to glasses, Chapters 14 and 15.

1.4 Non-spherical Particles

The last three decades have seen an extension of packing problems beyond sphere packing, to include hard particles of anisotropic shapes (Chapter 8), such as ellipsoids (Chapters 7 and 19), polyhedra (Chapters 8 and 9), or rods (Chapter 5), as well as soft or elastic bodies. Chapter 13 describes a number of imaging techniques to extract data from experimental samples.

In particular, the work by Donev *et al.*,[21] involving experiments with ~~el-lipsoidal-shaped~~ *M&M* ~~sweets~~, attracted the attention of many news broad-casters, such as the BBC and CNN. The Princeton group showed that ~~these sweets~~ pack closer than random arrangements of spheres (Bernal packing). Computer simulations revealed the dependence of packing density on the aspect ratio of the ellipsoids,[21] a result mirrored in two dimensions for the packing of ellipses.[22]

The exploration of tetrahedron packing has been another significant mathematical challenge. Conjectures for the densest packings have involved a combination of computational and theoretical methods, with significant breakthroughs occurring in recent decades due to the work of Torquato and Jiao[23] (Chapter 8) and by Chen *et al.*,[24] with the latter achieving the highest packing density of regular tetrahedra reported to date.

Advances in computer simulation techniques and software have resulted in an increasingly comprehensive and versatile approach to tackling packing problems, and revealed a veritable "zoo" of both ordered and disordered structures to explore and understand (Figure 1.7). Indeed, ~~advancements~~ in computer simulations now make it feasible to explore the dense packing of irregular, non-convex particles. This is achieved by approximating these com-plex particles with triangles, which simplifies the process of testing for over-laps. Such progress significantly broadens the scope of research in the field.[25]

The HOOMD-blue toolkit developed by the group of Sharon Glotzer[26,27] is one such general-purpose hard particle simulations toolkit. For the

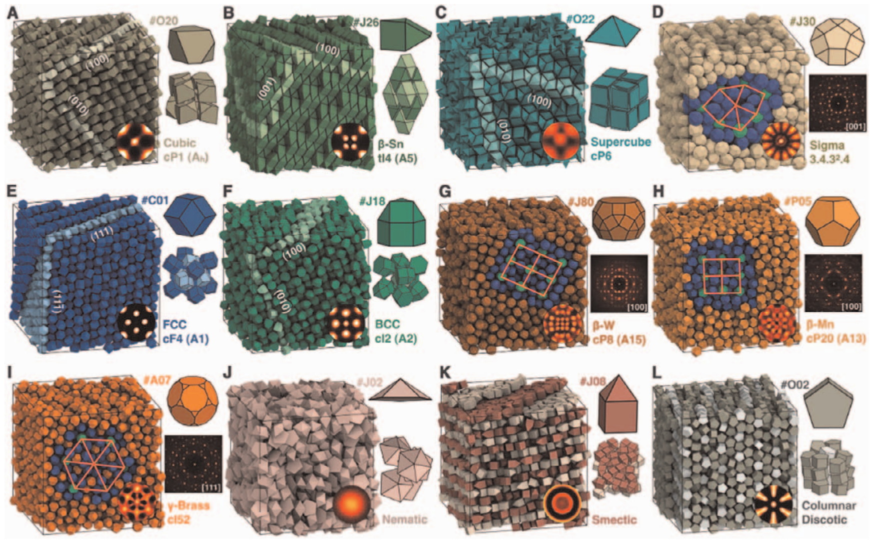


Figure 1.7 Hard polyhedral particles are observed to crystallize into distinct classes of matter: crystalline solids (types A–D), plastic crystals (types E–I), and liquid crystals (types J–L). The class type is primarily determined by the particular shape of the polyhedra that are being packed. For comprehensive details, see ref. 20. Reproduced from ref. 20 with permission from AAAS, Copyright 2012.

simulation of bubbles, Ken Brakke's Surface Evolver, published originally in 1992[28] and frequently updated,[29] continues to be the standard tool.

1.5 Amorphous Packings

Random and amorphous packings include macroscopic granular materials, such as sand, rice, and coffee granules, but are also linked to the structure of non-equilibrium, low-temperature amorphous phases of matter, which are essential for understanding phenomena ~~like~~ the glass transition[30] (Chapter 14).

Numerous experiments have explored the impact of friction between grains, often resulting in loosely packed structures[31] (Chapter 11). Investigations into amorphous sphere packings address the mechanical and flow behaviours of dense granular matter and uncovered universal features of the jamming transition from fluid to structurally arrested states.[32] Recent research has also delved into anisotropic packings of frictional grains induced by shear deformation, which leads to shear jamming[33] (see also Chapter 9). Efforts to comprehend the structure of these packings have incorporated concepts such as hyperuniformity[34] (Chapter 8), while more recently, machine learning techniques have been used to characterise various amorphous packings[35] (Chapter 16).

1.6 Confined Packings

Confinement within specific finite boundaries sometimes adds further complications. One example is the packing of equal-sized disks within polygonal boundaries. Imagine a scenario where circular disks of a fixed diameter need to be carved out of a square plate composed of any material, and with a predetermined side length. The essential question becomes: what is the maximum number of disks that can be extracted? The website http://www.packomania.com/, maintained by Eckard Specht from the University of Magdeburg, contains a vast collection of computed configurations (Figure 1.8).

Another intriguing variation in geometric packing is the arrangement of points or disks on a finite surface. This was first explored by Dutch botanist Paul L. Tammes in 1930 during his research on the distribution of stomata on pollen grains.[36] (See Figure 1.9 for an example.) Tammes was interested in finding the configuration that would maximize the separation between (equal-size) pores. The Tammes problem soon expanded beyond its biological context to become a significant mathematical challenge: it now focuses on optimally distributing a certain number of points on a sphere's surface to maximize the distance between any pair of points. Related to the Tammes problem is the Thomson problem of packing electrical *charges* on the surface of a sphere.[37] Symmetric arrangements of mutually repelling floating magnets in the presence of an external magnetic confining field were initially studied as a model system for atom arrangements in molecules[38] or the arrangements of electrons within an atom.[39] They continue to be examined in the general context of structure formation in confinement.[40]

Other variations on packing in confinement include the packing of spheres within a sphere,[41] or the packing of hard spheres (Chapter 2), or ellipses and spheroids (Chapter 3) in narrow channels. Chapter 4 describes phyllotactic patterns on a disk.

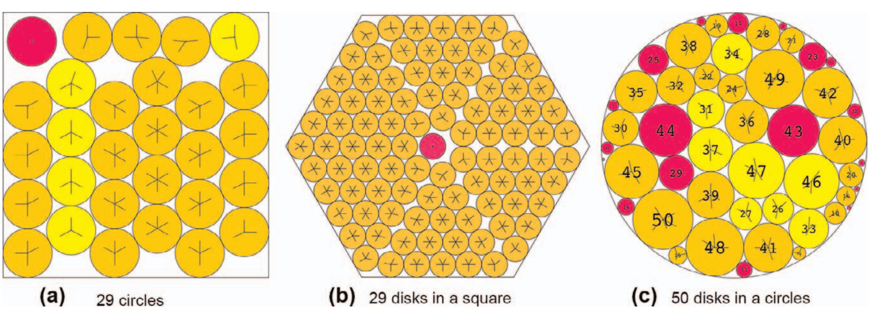


Figure 1.8 Densest packing of (a) 29 disks in a square, (b) 96 disks in a hexagon, and (c) 50 disks with incremental radii (the radii are integers from 1 to 50) in a circle. For more examples, see http://www.packomania.com/. Reproduced from http: //www.packomania.com/ with permission from E. Specht.

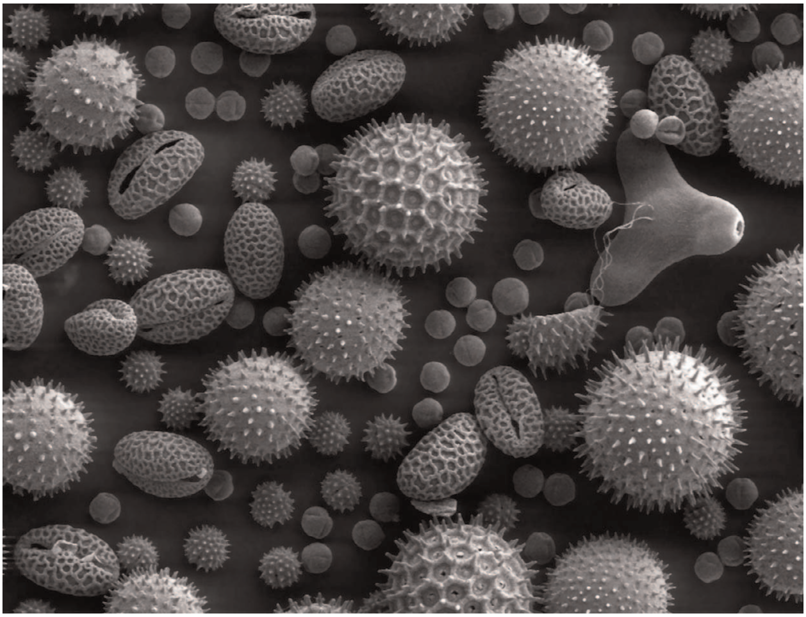


Figure 1.9 Scanning electron microscopic image of various pollen grains. A number of pollen grains can be interpreted as spheres on which circular pores are distributed evenly, ~~thus~~ the Tammes problem is one of packing non-overlapping disks as densely as possible on the surface of a sphere. Reproduced from https://svs.gsfc.nasa.gov/10394 with permission from NASA/Goddard Space Flight Center.

1.7 Recent Activities of the Packing Community: Geompack

A valuable perspective on a variety of cutting-edge developments can be gained by examining recent international meetings dedicated to packing problems, such as the “International Conference on Packing Problems”. This conference series was founded by ~~us~~ in 2012[42] and has since taken place five times in both Europe and the US.

We also highlight two other significant examples, with which we have been intimately involved. The first is a series of influential online meetings accessible at www.geompack.com. These virtual gatherings have been instrumental in fostering the growth of the field. Following on from this, the second is a month-long Satellite Programme of the Isaac Newton Institute, held in Abersywtyth University in 2023, titled “GeomPack: Geometry and Packing in Material Structure and Biology”. Video recordings of the invited presentations are found at https://www.youtube.com/playlist?list=PLGYCoKMjmerf4uNZ7cQ1AXxOx_k4TOPPH.

For readers daunted by the extensive detail, a more accessible entry point is offered by Aste and Weaire’s “The Pursuit of Perfect Packing”.[13] This book presents an easy-to-follow introduction to the field, ideal for beginners.

1.8 The Present Volume

The subsequent chapters of this book aim to provide a comprehensive snapshot of the field as it currently stands. The material presented is grouped in two parts. Part A is dedicated to theory and modelling of packing problems, covering both ordered (Section ~~1.~~1) and disordered (Section ~~1.~~2) arrangements.

In Part B, packing problems are described according to the length scales which are involved in specific contexts. This ranges from centimetres to tens of microns in the case of foams and granular matter (Section ~~1.~~3), several hundred nanometres, as in amorphous materials (Section ~~1.~~4) and colloids (Section ~~1.~~5), down to the nanoscale (Section ~~1.~~6).

Each chapter is written by experts who provide an overview of their specific field, together with comprehensive lists of references that invite us to dig deeper.

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