Short-course on symmetry and crystallography

Introduction

Michael Engel
Ann Arbor, June 2011
Books

- **Sands**: Introduction to crystallography (Dover Classics)
  Very good summary, short, cheap.

- **Weyl**: Symmetry (Princeton)
  Classic, written for non-scientists, bed-time read.

- **Massa**: Crystal structure determination (Springer)
  For crystallographers working with atomic crystals, if you are interested in details.

- **Hahn**: International tables for crystallography, Volume A (space group symmetry) For reference.

No (modern) textbook covering all the topics.
Symmetry (from the Greek: "συμμετρεῖν" = to measure together), generally conveys two primary meanings.

1. Symmetry is an imprecise sense of harmonious or aesthetically pleasing proportionality and balance; such that it reflects beauty or perfection.

2. Symmetry is a precise and well-defined concept of balance or "patterned self-similarity" that can be demonstrated or proved according to the rules of a formal system: by geometry, through physics or otherwise.

Wikipedia entry on “Symmetry”
**Beauty:** Architecture (Taj Mahal)

**Design/Photography** (golden mean)

**Small:** Elementary particles (spin 1/2)

- $s = 0$
- $s = -1$
- $s = -2$

**Big:** Galaxies (Whirlpool and Sombrero)
Importance of symmetry

• Symmetry “pleases the eye”.

• Symmetry counters disorder/chaos.

• Symmetric solutions are (often) the correct ones.

• “Symmetric objects” and “symmetric materials” are more attractive for applications. (?)

• Too much symmetry can be boring (artificial?).
**Art:** Islamic tilings for decoration

**Nature:** Sunflower (fractals and spirals)

**Uniformity:** Gypsum (Chihuahua, Mexico)

**Artificial:** Silicon single crystal (> 99.99999% Si)
Quasicrystal: icosahedral-YbCd

Atomic crystal: Clathrate hydrates

Morphology: Water ice

Self-assembly: hard tetrahedra
In a tale that has risen to legend in the field, Seeman was drinking a beer in a bar in Albany when an image of the M. C. Escher woodcut *Depth* popped into his head. The woodcut depicts dozens of flying fish soaring in formation [...]. Seeman realized that artificial DNAs with [...] could be tailored to link up into a regular 3D cubic lattice [...]. And as a crystallographer, Seeman immediately envisioned that such an array could be used to trap copies of a single protein in the voids and get them to line up with the same orientation. In other words, he imagined a tool for determining the structure of virtually any protein at will.
Outline

• **Point symmetry**
  Groups, point groups, Hermann-Mauguin and Schoenflies notation, permutation group (?), group representation (?).

• **(Periodic) Lattices**
  Unit cell, crystal systems, Bravais lattices, tilings, quasicrystals.

• **Crystals**
  Space groups, International Tables for Crystallography, online resources and space group identification.

• **Diffraction patterns**
  Fourier transformation, structure factor, X-ray, neutron and electron diffraction, crystal defects
What should you (hopefully) be able to do after four weeks?

- Determine a point group of an object by hand
- Determine a space group using internet resources
- Understand symmetry notations in papers
- Read Wikipedia articles like “Group_(mathematics)”, “Space_group”, ...
- Extract the information contained in diffraction patterns
The Free-Energy Landscape of Clusters of Attractive Hard Spheres

Guangnan Meng, Natalie Arkus, Michael P. Brenner, Vinothan N. Manoharan

Fig. 3. (A) Optical micrographs and renderings of nonrigid structures at $N = 9$ (see also movies S2 and S3) and (B) $N = 10$ (movies S4 to S6). (C) Structures of $3N - 5 = 25$ bond packings at $N = 10$ (movies S7 to S9). The anharmonic vibrational modes of the nonrigid structures are shown by red arrows. Experimentally measured probabilities are listed at top. Annotations in micrographs indicate clusters corresponding to subsets of HCP or FCC lattices. Scale bars, 1 µm.
Quasicrystalline order in self-assembled binary nanoparticle superlattices

Dmitri V. Talapin\textsuperscript{1,2*}, Elena V. Shevchenko\textsuperscript{2*}, Maryna I. Bodnarchuk\textsuperscript{1}, Xingchen Ye\textsuperscript{3}, Jun Chen\textsuperscript{4}
& Christopher B. Murray\textsuperscript{3,4}
Refinement of the crystal structure of \( \alpha \)-silicon tetrabromide, \( \alpha \)-SiBr\(_4\), a room temperature modification

Abstract
Br\(_4\)Si, \( Pa\bar{3} \) (no. 205), \( a = 11.152(1) \) Å, \( V = 1386.9 \) Å\(^3\), \( Z = 8 \), \( R_g(F) = 0.046 \), \( wR_{ref}(F^2) = 0.087 \), \( T = 223 \) K.

Table 1. Data collection and handling.

<table>
<thead>
<tr>
<th>Crystal:</th>
<th>colorless cube, size 0.3 × 0.3 × 0.3 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wavelength:</td>
<td>Mo ( K_\alpha ) radiation (0.71073 Å)</td>
</tr>
<tr>
<td>( \mu ):</td>
<td>232.52 cm(^{-1})</td>
</tr>
<tr>
<td>Diffractometer, scan mode:</td>
<td>STOE IPDS II, ( \omega )</td>
</tr>
<tr>
<td>( 2\theta_{max} ):</td>
<td>39.96°</td>
</tr>
<tr>
<td>( N(hkl)<em>{measured}, N(hkl)</em>{unique} ):</td>
<td>4180, 215</td>
</tr>
<tr>
<td>Criterion for (I_{obs} ), ( N(hkl)_{gt} ):</td>
<td>( I_{obs} &gt; 2 \sigma(I_{obs}) ), 188</td>
</tr>
<tr>
<td>( N(param)_{refined} ):</td>
<td>17</td>
</tr>
<tr>
<td>Programs:</td>
<td>SHELXS-97, SHELXL-97 [7]</td>
</tr>
</tbody>
</table>

Table 2. Atomic coordinates and displacement parameters (in Å\(^2\)).

<table>
<thead>
<tr>
<th>Atom</th>
<th>Site</th>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Br(1)</td>
<td>8c</td>
<td>0.2448(1)</td>
<td>( x )</td>
<td>( x )</td>
</tr>
<tr>
<td>Br(2)</td>
<td>24d</td>
<td>0.0244(3)</td>
<td>0.0123(2)</td>
<td>0.2450(1)</td>
</tr>
<tr>
<td>Si(1)</td>
<td>8c</td>
<td>0.1313(2)</td>
<td>( x )</td>
<td>( x )</td>
</tr>
</tbody>
</table>
Entropic Stabilization of Tunable Planar Modulated Superstructures

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(Received 8 November 2010; published 2 March 2011)
Not covered

- Continuous symmetries, lie groups
- Spherical harmonic (hydrogen problem)
- Crystal structure refinement
- Symmetry and conservation laws (Noether’s theorem)
- Symmetry breaking
- ...