PHSX 886: Homework #1

September 8, 2025

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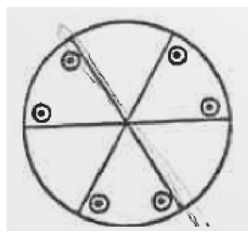
Problem 1

Show that the $\bar{6}$m2 point group symmetry can be represented by the following stereographic projection:

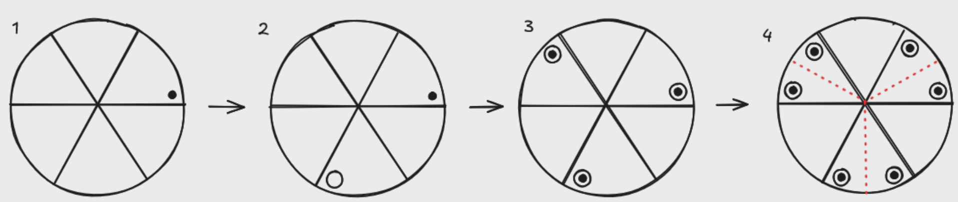


In your answer, please begin with a single direction (one of the dots on the above figure). Then, show how each symmetry operation can produce other equivalent directions in the figure.

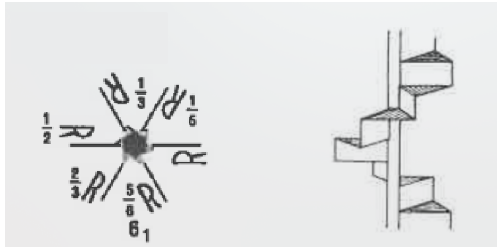
(Note: the 6 axis is along the out-of-plane (z) direction; the m represents mirror plane perpendicular to the x, y, u directions; the ”2” represents 2-fold rotation axis along the $\langle 110 \rangle$ type direction).

Solution:

1. Begin with a point at a single, arbitrary direction in a stereographic projection, such as $\langle 101 \rangle$ (assume any cell shape).
2. We can reach the nearest neighbor point on the circle with a rotation by 60° along the axis into the paper. This is then inverted under the transformation $r \to -r$.
3. This is repeated 6 times total, such that we arrive back at the starting point.
4. Finally, this is mirred across the 2-fold rotation axis in the $\langle 110 \rangle$ direction.



Problem 2



Which symmetry element can produce a left-handed version of the above structure?
In your answer, please show/explain, step-by-step, how the symmetry you stated can produce left-handed spiral structure.

Solution:
If we were to construct a right-handed structure, given above, we would use $\mathrm{P6}_1$. Each step, going around the circle would be at: $\{0, 1/6, 2/6, 3/6, 4/6, 5/6\}$.

The right-handed structure is instead given by $\mathrm{P6}_5$, producing steps at: $\{0, 5/6, 4/6, 3/6, 2/6, 1/6\}$.

These are related to each other by a mirror transformation across a plane, such as $(x, y, z) \to (x, -y, z)$.

Problem 3

Prove that the interplanar distance for a tetragonal crystal can be written as:

$$d(hk\ell) = \frac{1}{\sqrt{\frac{h^2+k^2}{a^2} + \frac{\ell^2}{c^2}}}$$

In this equation, h, k, ℓ are the Miller indices for the (hkℓ) plane.

Solution:
In a tetragonal cell, we have $|\vec{a}_1| = |\vec{a}_2| \neq |\vec{a}_3|$. Let $a = |\vec{a}_1| = |\vec{a}_2|$, and $b = |\vec{a}_3|$. Then, $\vec{g}_{hk\ell}$ will simplify to:

$$\vec{g}_{hk\ell} = \frac{1}{a}\left(h\hat{x} + j\hat{k}\right) + \frac{1}{\ell}\left(k\hat{z}\right)$$

$d_{hk\ell}$ is related to $\vec{g}_{hk\ell}$ by:

$$\begin{aligned} d_{hl\ell} &= \frac{1}{|\vec{g}_{hk\ell}|} \\ &= \frac{1}{\sqrt{\frac{h^2+k^2}{a^2} + \frac{\ell^2}{c^2}}} \end{aligned}$$

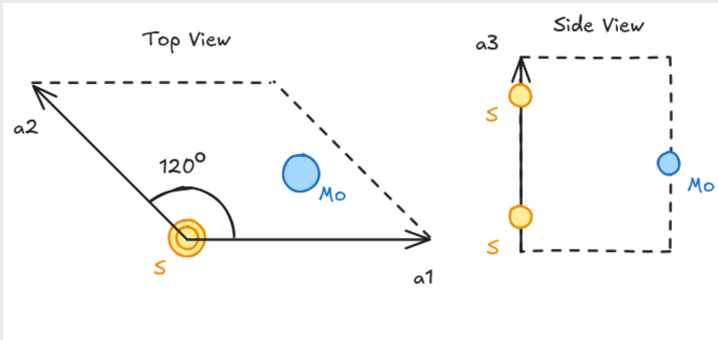
Problem 4

You can search online or from literature to find out how the MoS_2 crystal structure looks like and complete this question.

(a) Draw the unit cell for the monolayer MoS_2 structure. Define a valid set of lattice vectors and basis atoms.

Solution:

$\mathrm{MoS_2}$ has a $\mathrm{P\bar{6}m2}$ structure. This indicates that it is hexagonal with $\alpha = 90°$, $\beta = 90°, \gamma = 120°$.



I will choose a basis:

$$(\vec{a}_1 = 3.12\hat{x}, \vec{a}_2 = -1.6\hat{x} + 2.8\hat{y}, \vec{a_3} = 18.1\hat{z})$$

(b) Monolayer MoS_2 has a $\mathrm{P\bar{6}m2}$ space group (see also question 1). Does the crystal contain any inversion center? Hint: you can look at the figure in question 1, or the monolayer MoS_2 crystal itself.

Solution:

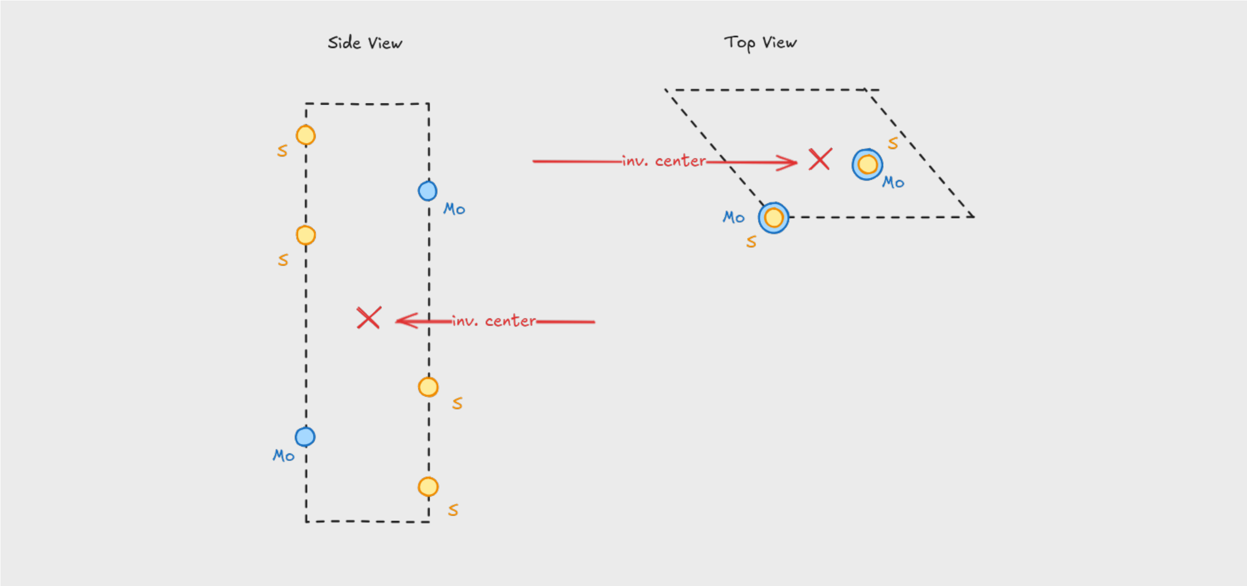
There is a rotoinversion symmetry for monolayer $\mathrm{MoS_2}$, but there is no inversion center. The presence of the lone Mo atom inside the cell breaks this symmetry.

(c) Does bilayer MoS_2 (the 2H phase) have an inversion symmetry? Draw the top and side view of the bilayer MoS_2 crystal and indicate where the inversion center is located.

Solution:

Bilayer $\mathrm{MoS_2}$ is inversion symmetric. When adding the second layer to the structure, symmetry is restored by the addition of the extra Mo atom and the mirror perpendicular to the c-axis. The inversion center sits between the two layers.

Problem 4 continued on next page...



(FYI, bilayer and bulk MoS_2 has a space group symmetry of $P6_3/mmc$ – No. 194)
Note: The presence or absence of inversion center can lead to drastic change in non-linear optical properties when one changes the number of layers. See e.g.,
Phys. Rev. B 87 161403(R), 2013 (Research done in Prof. Zhao's group at KU.)