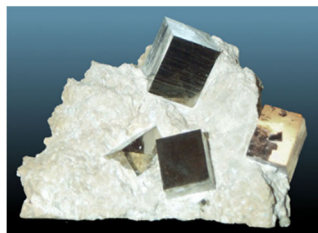
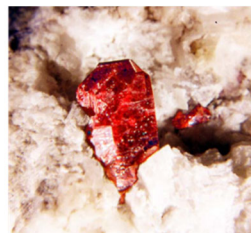
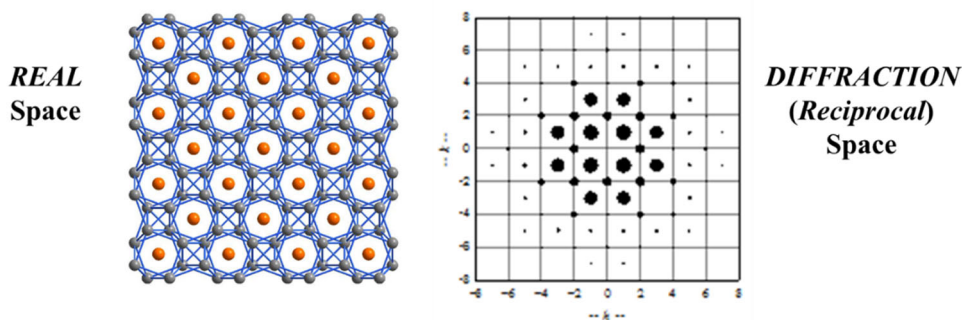


STRUCTURAL SYMMETRY OF CRYSTALS

(3) **Macroscopic vs. Microscopic Features:** Crystalline symmetry reveals itself over length scales ranging from macroscopic to microscopic. Crystals form well-defined faces, sharp edges, and interfacial angles that adopt specific values depending on the overall symmetry of the solid. These features are evident in the figures of pyrite and cinnabar crystals.¹ The macroscopic shapes of crystals arise from the microscopic arrangements of the constituent atoms. Amorphous or noncrystalline solids generally lack these macroscopic features, as exemplified by the white material in which the crystals are embedded. Examples of noncrystalline substances include glasses, gels, and some nanostructured materials.

Pyrite (FeS_2): CubicCinnabar (HgS): Trigonal

Any atomic structure that repeats periodically in space will give rise to a diffraction pattern obtained using X-ray, electron, or neutron scattering. By analyzing the pattern for the relative locations and intensities of the peaks (spots or lines), the atomic structure of the crystal can be solved. Atomic structure, which is described by bond distances and bond angles based on atomic positions, occurs in *real space*, whereas diffraction patterns are mapped out in *reciprocal space*, where distances between points have units 1/length, e.g., $1/\text{\AA}$ or $1/\text{nm}$. Nevertheless, the symmetry of the diffraction pattern in reciprocal space always mimics the symmetry of the atomic (crystal) structure in real space.

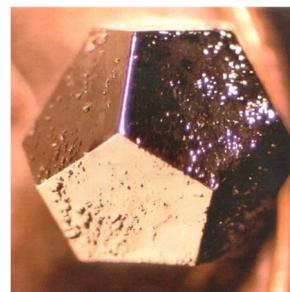


- (4) Therefore, crystalline symmetry involves two components:
- (1) *translational*, which is described by a lattice of points that repeat periodically throughout real space; and
 - (2) *rotational*, which is specified by rotation axes and reflection (mirror) planes and is determined by the short-range and long-range organization of atoms of the structure.

These two symmetry components are not mutually exclusive. Taken together, they are used to constitute *space groups*.

¹ Images at <http://webmineral.com>, © David Bethelmy.

In the mid-1980s, Shechtman et al. reported icosahedral symmetry in electron diffraction patterns for a Mn-Al alloy,² but this point symmetry cannot occur exactly in a crystal. This discovery elicited much discussion about the types of solid-state structures that give diffraction patterns. Ultimately, this Mn-Al alloy was called a *quasicrystal*, which is neither crystalline nor amorphous. Since that report, hundreds of quasicrystals have been synthesized and characterized, such as the one shown here, which was prepared in the Ames Laboratory for a Y-Mg-Zn alloy.³ Although most quasicrystals have been prepared in a laboratory, natural quasicrystals have been identified in meteorites, such as icosahedrite ($\text{Al}_{63}\text{Cu}_{24}\text{Fe}_{13}$)⁴ and decagonite ($\text{Al}_{71}\text{Ni}_{24}\text{Fe}_5$),⁵ which show decagonal (10-fold) symmetry.



Y-Mg-Zn quasicrystal prepared in the Ames Laboratory (ISU) by I. Fisher, P. Canfield et al.

An important coupling of the macroscopic and microscopic characteristics of symmetry in solids is *Neumann's Principle*, which states that the macroscopic (tensor) properties of a crystal have at least the symmetry of the *point group of the space group*. Another statement of this principle is that if a crystal is invariant with respect to certain rotational symmetry, then any of its physical properties must also be invariant with respect to the same rotational symmetry. The consequences of Neumann's Principle are significant and emphasize the importance of a thorough structural characterization of matter.

² Shechtman, D.; et al. *Phys. Rev. Lett.* **1984**, *53*, 1951-1953.

³ Fisher, I.R.; et al. *Philos. Mag. B* **1998**, *77*, 1601-1615.

⁴ Bindi, L.; et al. *Proc. Natl. Acad. Sci.* **2012**, *109*, 1396-1401.

⁵ Bindi, L.; et al. *Amer. Miner.* **2015**, *100*, 2340-2343.