Quasicrystals: An Overview

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Metallic Phase with Long-Range Orientational Order and No Translational Symmetry

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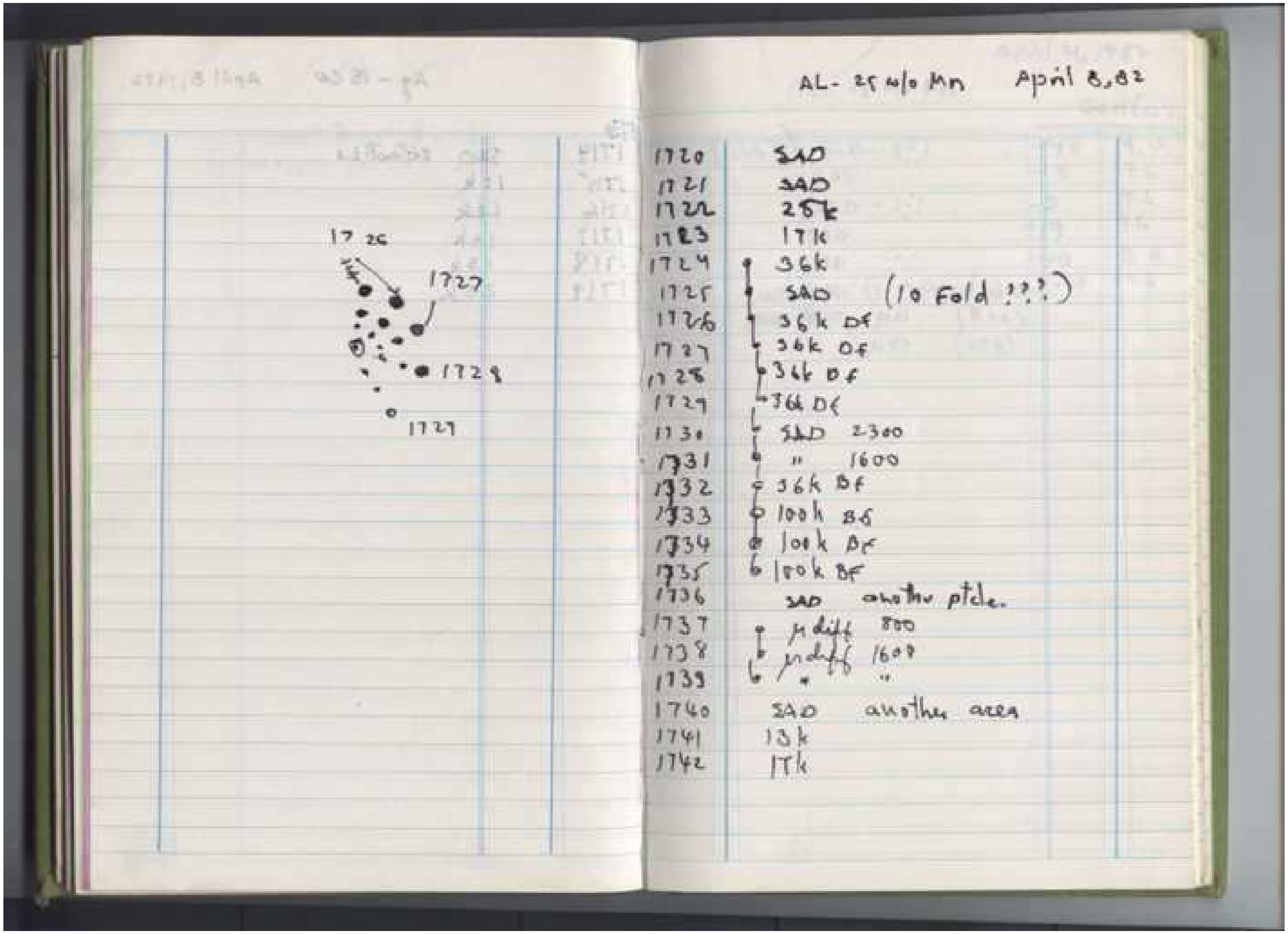
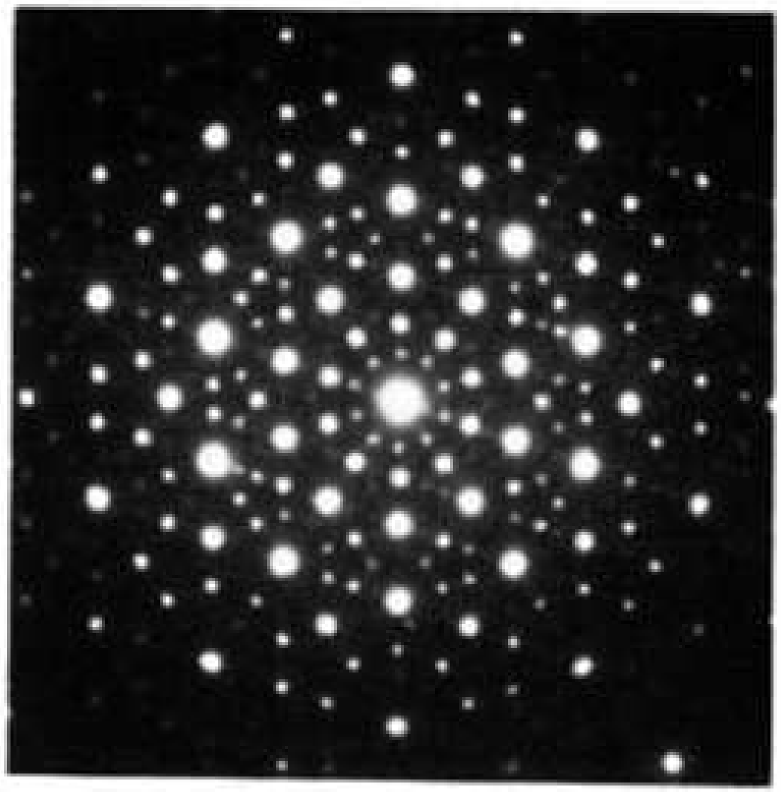
We have observed a metallic solid (Al–14-at.%-Mn) with long-range orientational order, but with icosahedral point group symmetry, which is inconsistent with lattice translations. Its diffraction spots are as sharp as those of crystals but cannot be indexed to any Bravais lattice. The solid is metastable and forms from the melt by a first-order transition.

PACS numbers: 61.50.Em, 61.55.Hg, 64.70.Ew

Shechtman's Experiment



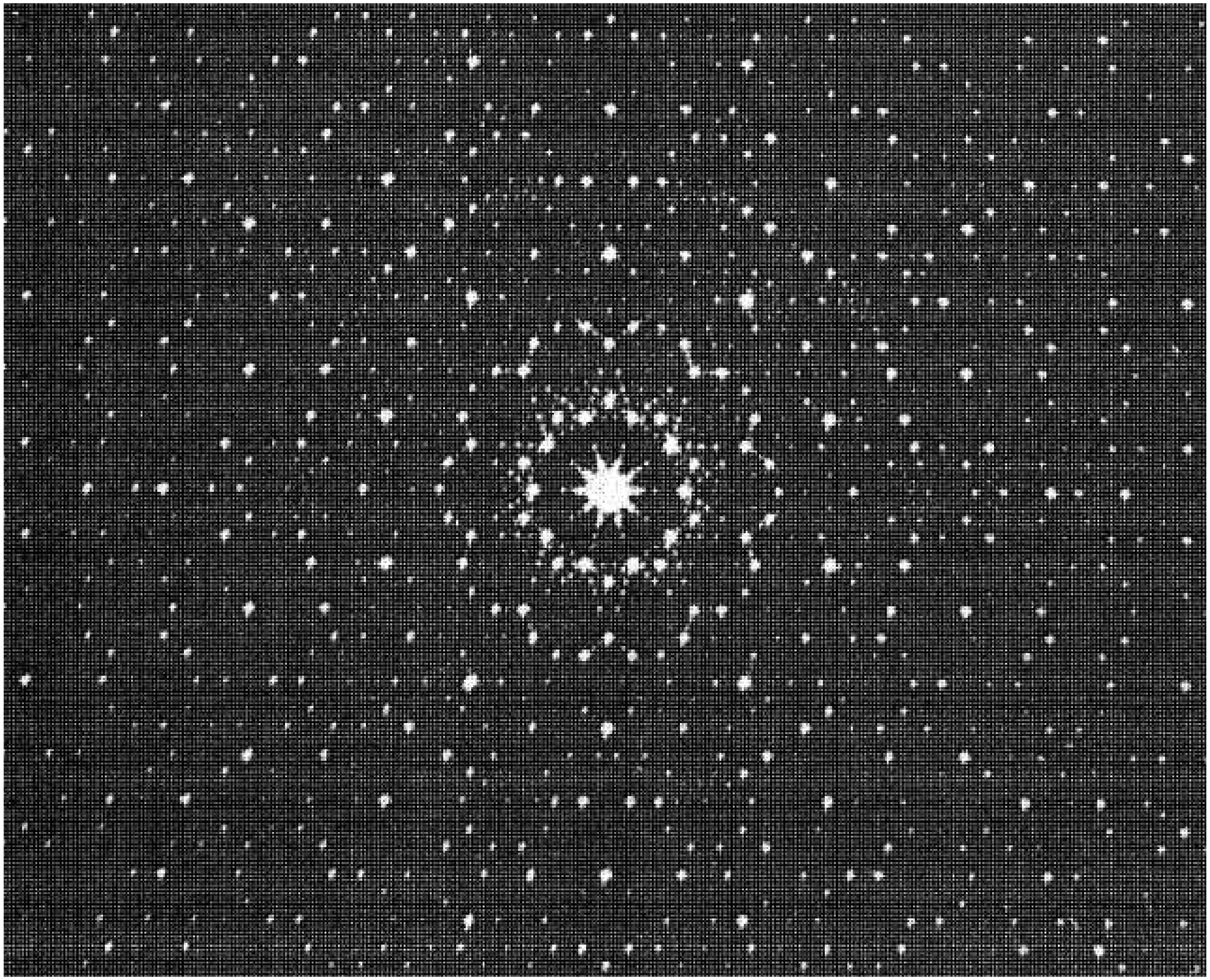
Sharp Diffraction Peaks, 10-fold Symmetry



- electron diffraction pattern
- rapidly quenched Al-Mn alloy
- sharp diffraction spots,
  like a crystal
- 10-fold symmetry,
  so can't be a crystal!
- what can this be???

Twinned crystals can be ruled out by selected area diffraction and high resolution imaging.

Diffraction Pattern of Penrose Tiling



A. Mackay, Physica **114**A, 609–613 (1982)

Al-Mn Quasicrystal has Icosahedral Symmetry

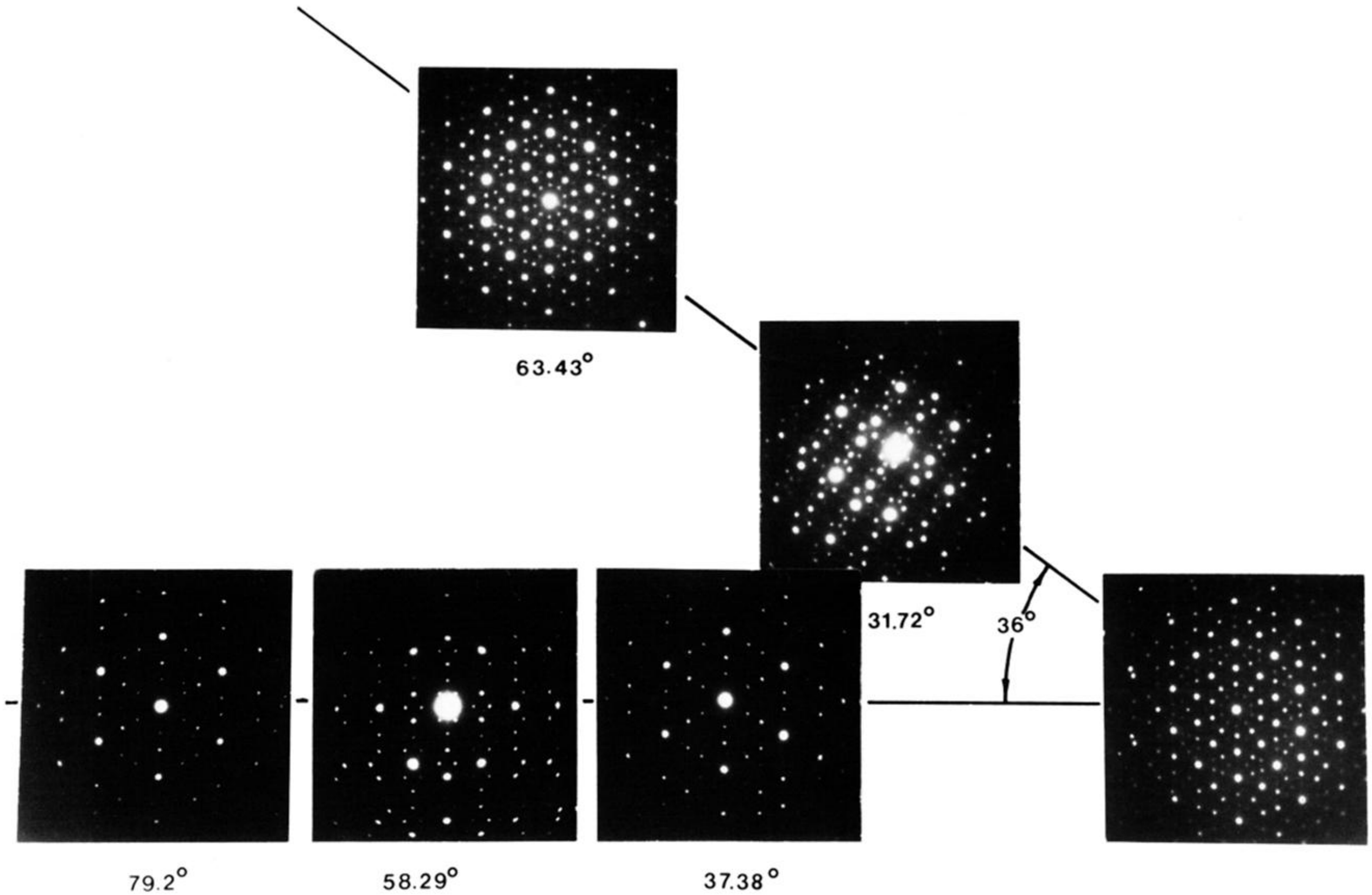


FIG. 2. Selected-area electron diffraction patterns taken from a single grain of the icosahedral phase. Rotations match those in Fig. 1.

Today: Much Better Samples

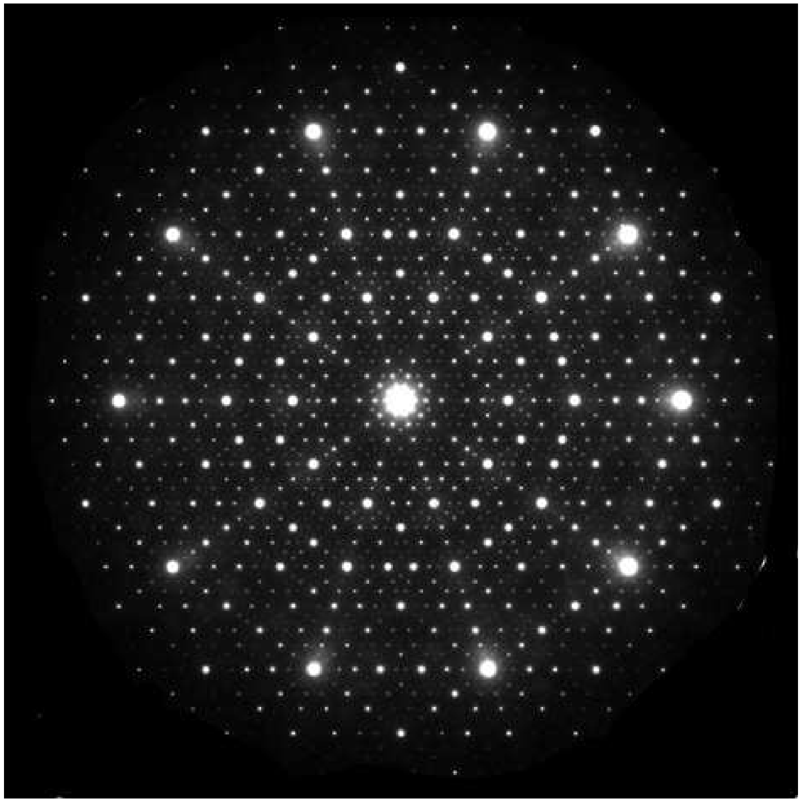


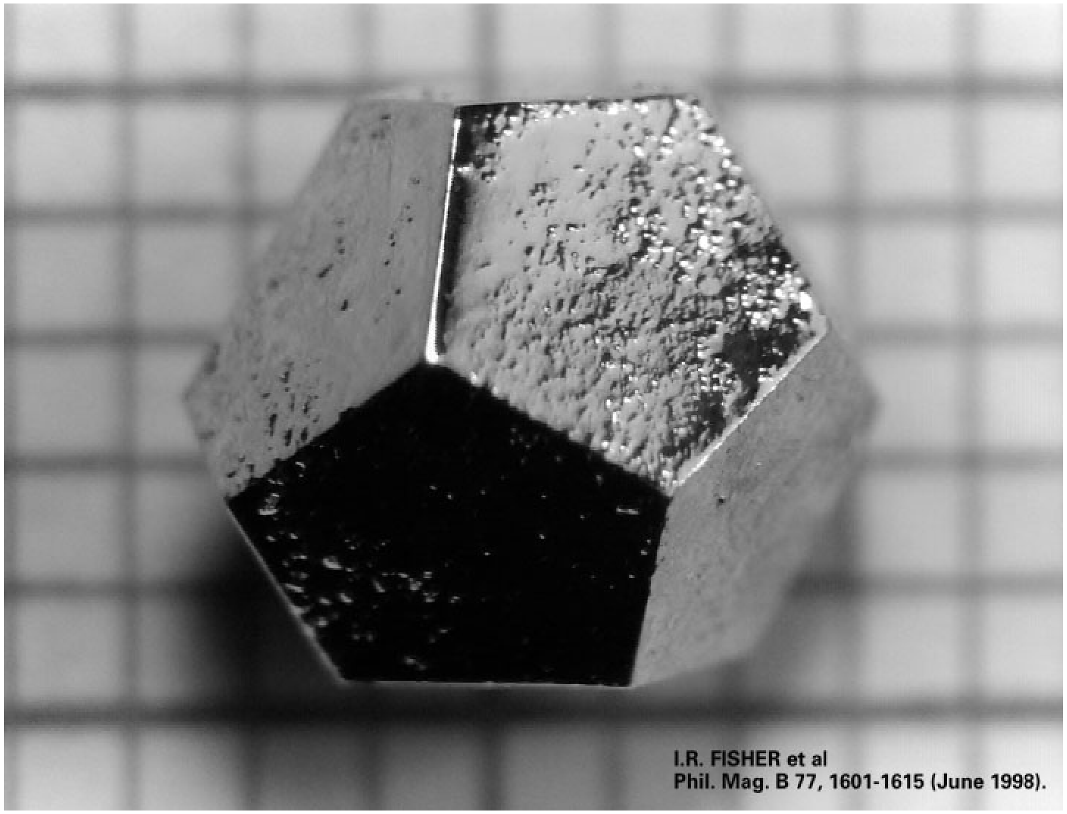
Image: C. Beeli

- several big families
- icosahedral Al-Pd-Mn, Al-Cu-Fe, Zn-Mg-RE, Cd-Ca, Cd-Yb, Zr-Ni-Ti, ...
- decagonal Al-Ni-Co, Al-Cu-Co, Al-Pd-Mn, ...
- octagonal and dodecagonal symmetry

Many quasicrystal phases are thermodynamically stable, at least at high temperature.

Morphology

Often, mm- or even cm-sized single-quasicrystals can be grown. Non-crystallographic symmetry visible in morphology:



Quasiperiodicity

Quasicrystals are quasiperiodic: density formally given by Fourier series

$$\rho(\mathbf{x}, \mathbf{x}^{\perp}) = \sum_{\mathbf{h} \in \mathbb{Z}^n} a_{\mathbf{h}} \, e^{i \sum_j h_j (\mathbf{k}_j + \mathbf{k}_j^{\perp}) \cdot (\mathbf{x} + \mathbf{x}^{\perp})}$$

with $n > d$ rationally independent basis vectors $\mathbf{k}_j$

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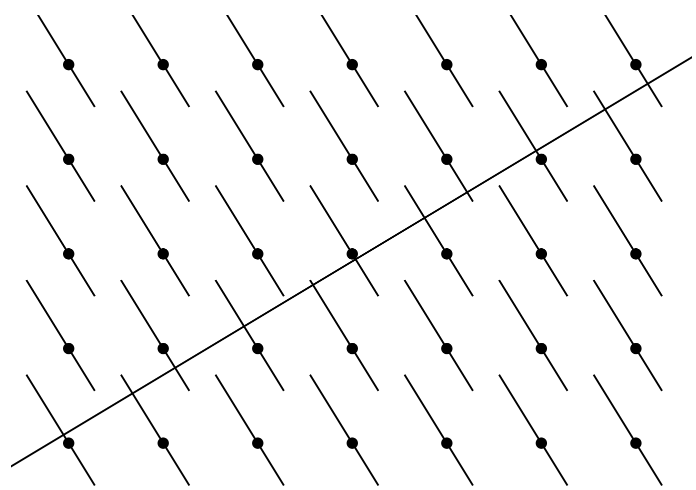
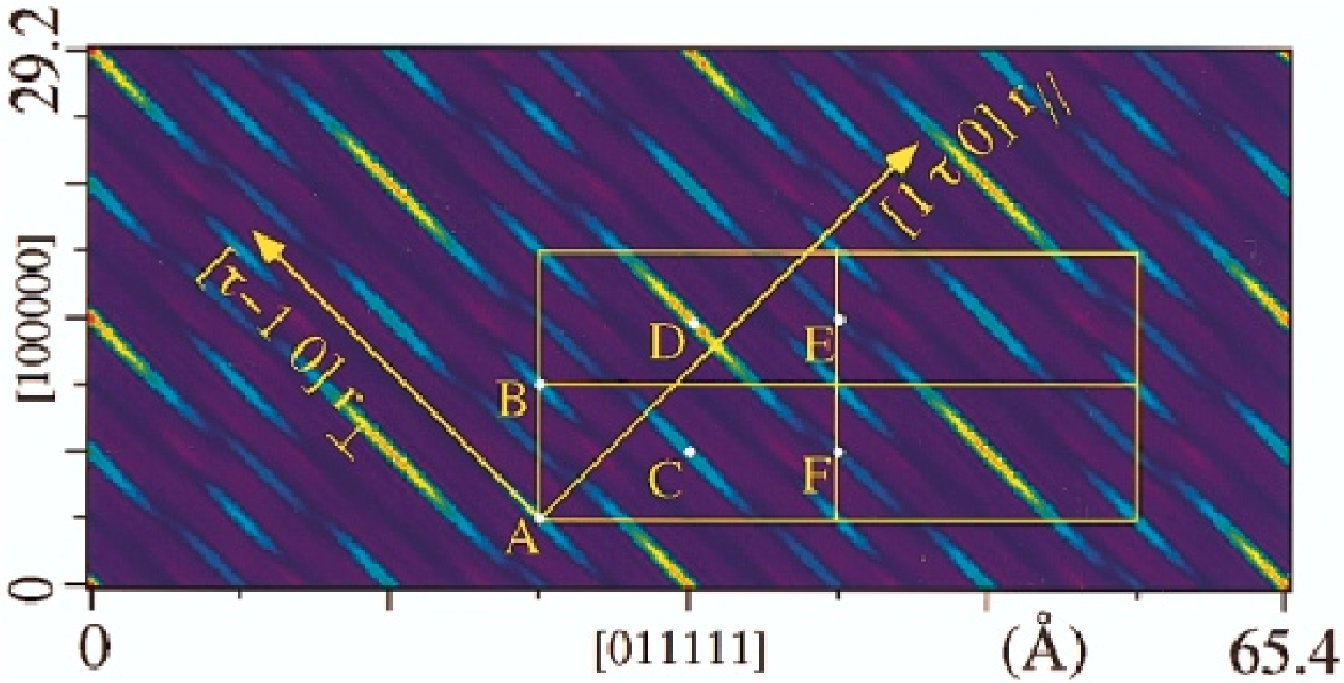
In real space: cut through n-dimensional crystal:



Structure Determination

Reconstructed electron density in 5-fold plane of i-ZnMgHo:



(H. Takakura et al., Phys. Rev. Lett. **86**, 236 (2001))

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Due to limited resolution, sharp boundaries of atomic surfaces are not measurable.

Diffraction Techniques

Neutron diffraction

- sees only nuclei
- differentiates between different isotopes
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X-ray diffraction (also by synchroton radiation)

- sees electron density, concentrated near heavy nuclei
- stronger coupling, but still weak enough for kinematic treatment
- main work horse for quantitative studies

Diffraction Techniques

Electron diffraction

- sees projected electrostatic potential
- very strong coupling
- tiny samples have to be used, but still multiple scattering (non-linear effects)
- quantitative information difficult to obtain,
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Diffraction measures averaged structure, giving split positions, partial or mixed occupancies, ... Further modelling required!

Imaging Techniques

High resolution Transmission Electron Microscopy:

- direct observation of structure and order
- sometimes difficult to interpret
- works best when looking along periodic direction (decagonal quasicrystals)

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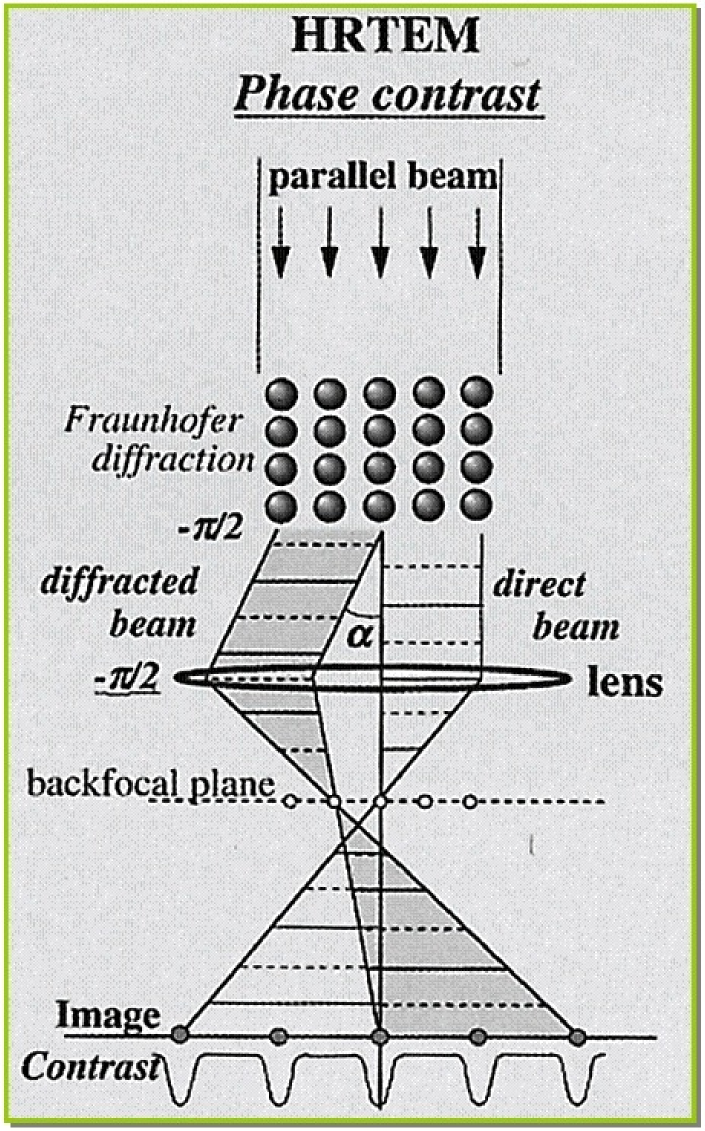
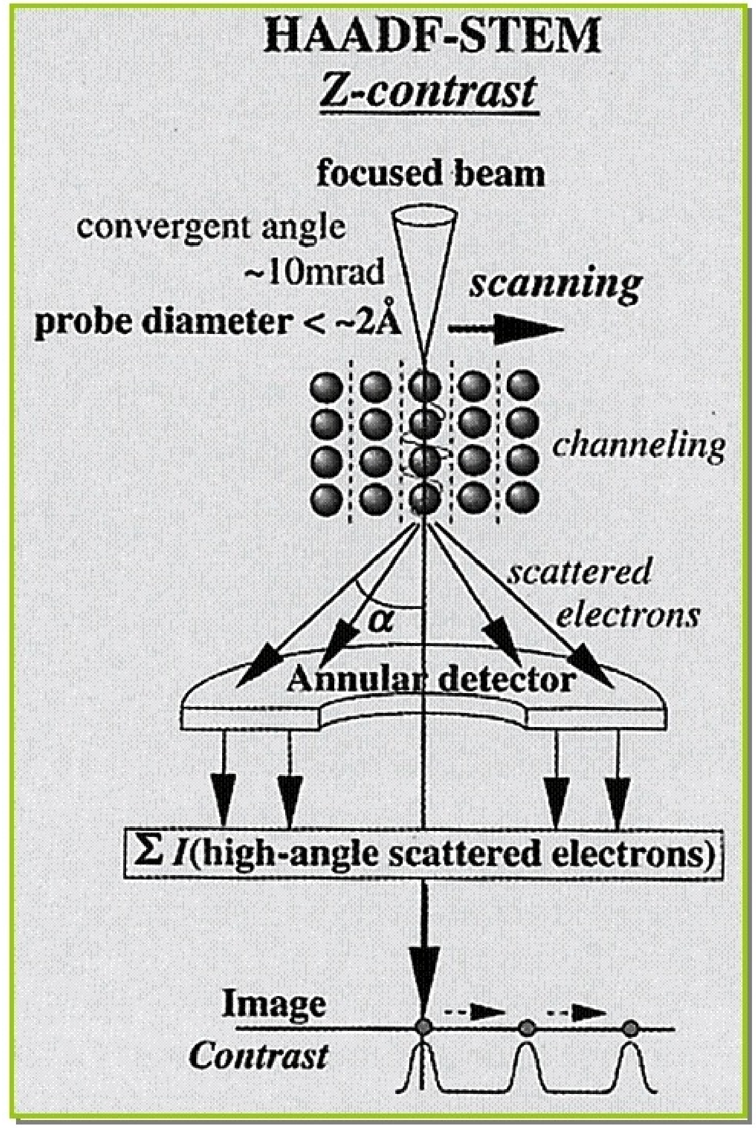
Surface techniques:

- scanning tunneling microscopy
- atomic force microscopy
- works only at surfaces
- surface structure may differ from interior

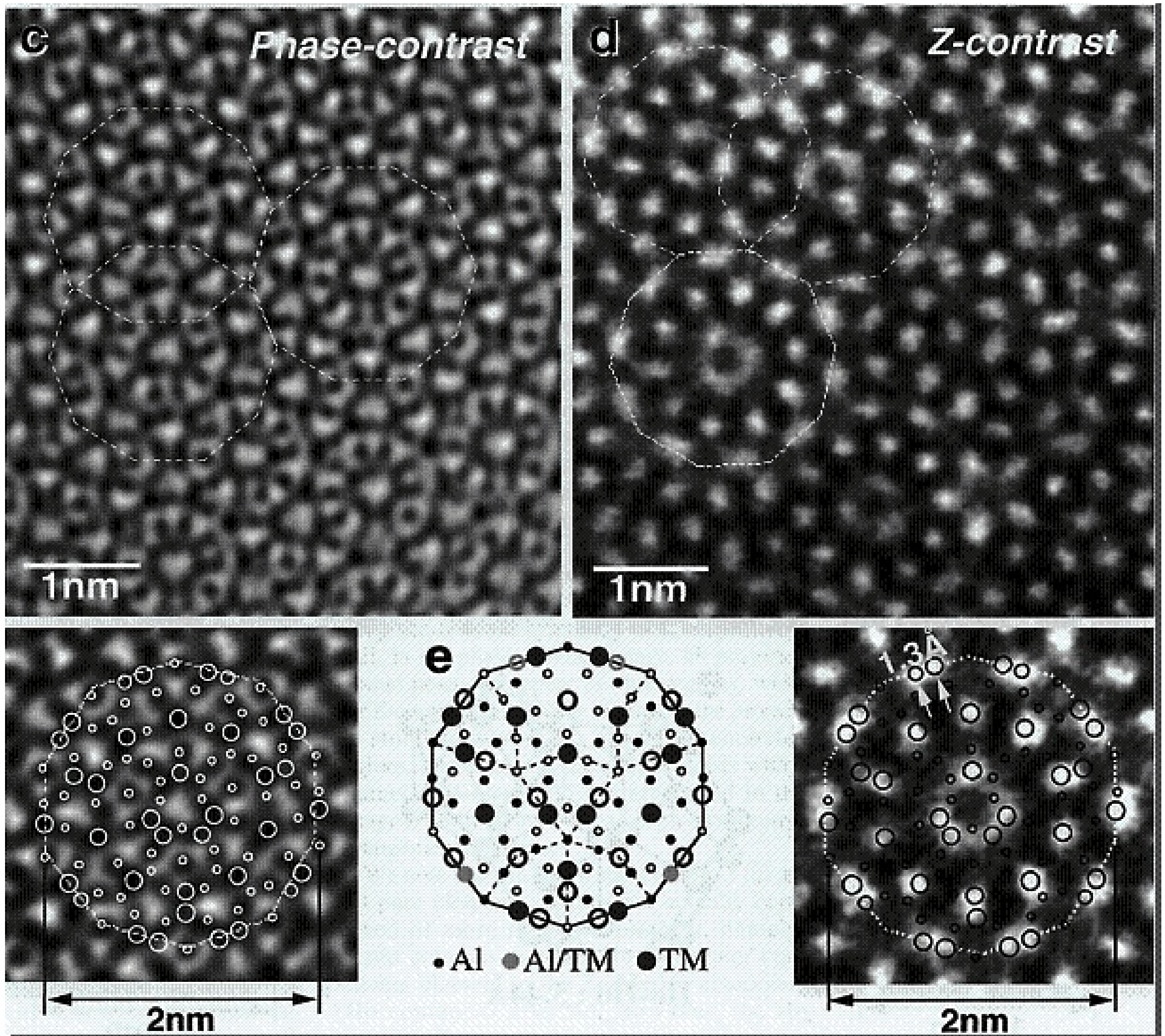
HRTEM versus HAADF-STEM





Abe & Tsai, JEOL News 36 (2001) 18)

Comparison HRTEM versus HAADF-STEM



Abe & Tsai, JEOL News 36 (2001) 18)

Direct Structure Imaging

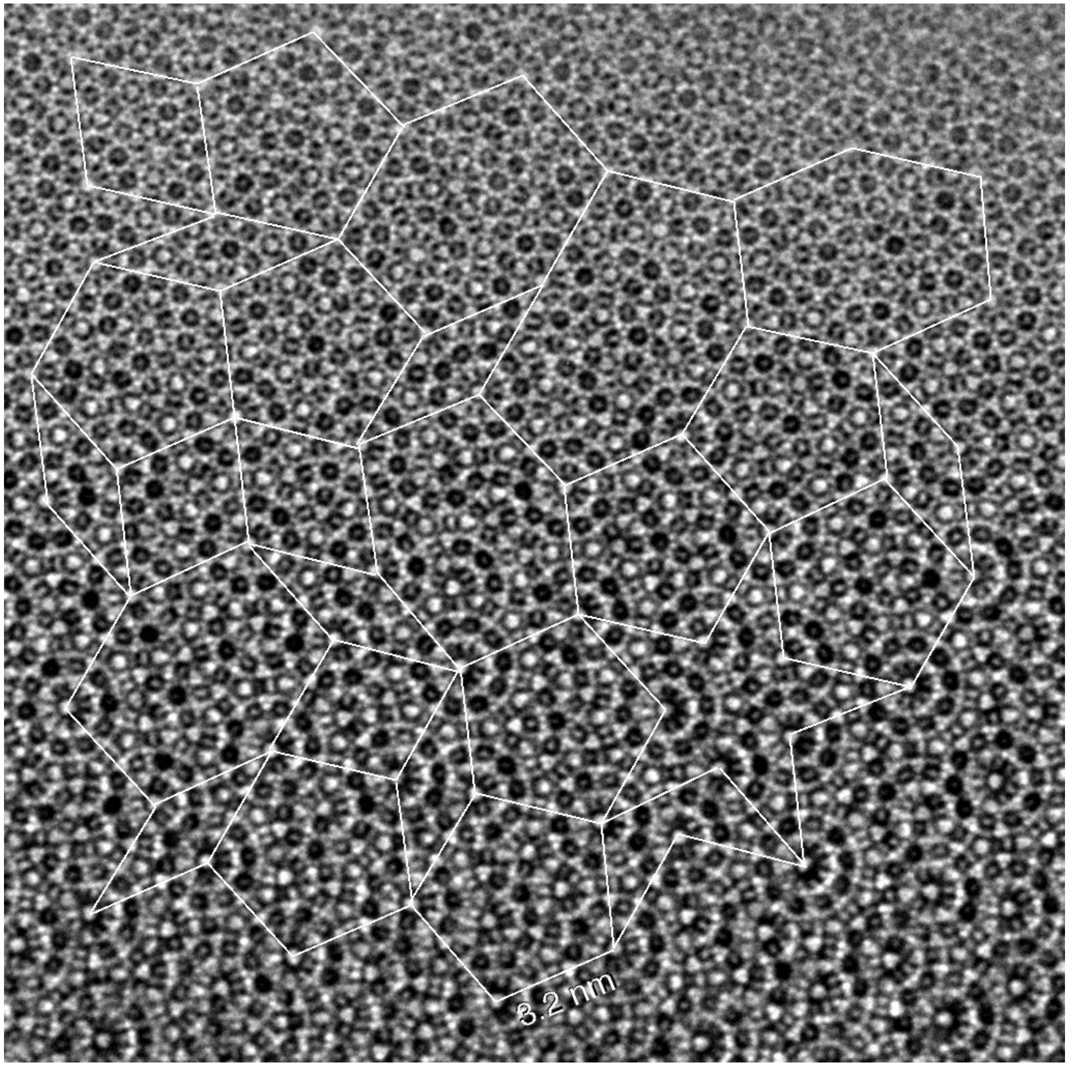
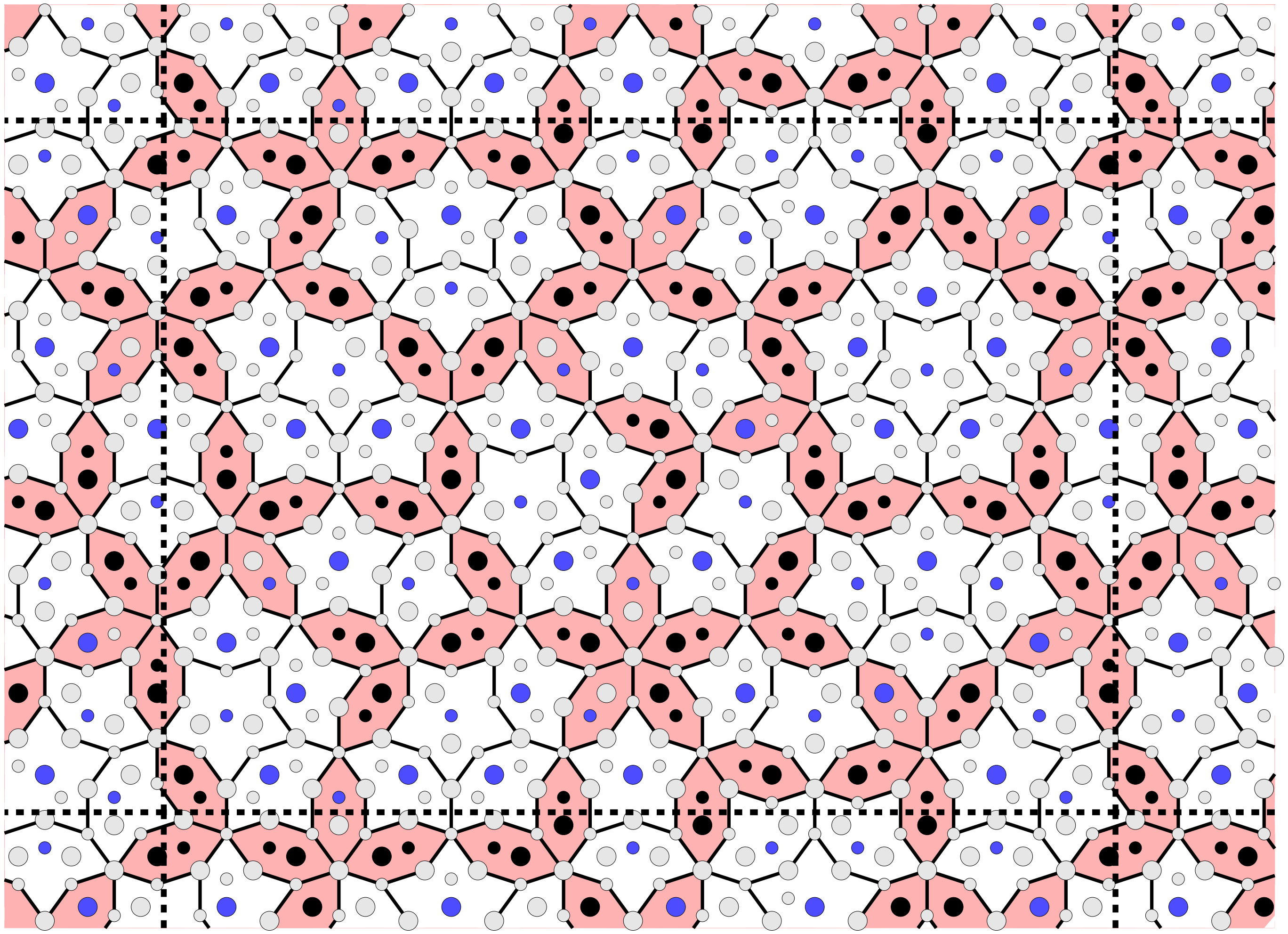


Image: S. Ritsch

Quasicrystals as Decorated Tilings



M. Mihalkovic et al.

Quasicrystals as Decorated Tilings

Decorated tiling models are highly desirable!

This allows to reshuffle tiles, play with structure variants, make periodic approximants.

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This allows to reshuffle tiles, play with structure variants, make periodic approximants.

Decorated tilings are an idealization, however.

Often, it is not clear what tiling to take.

Often, no tiling with simple decoration seems to exist.

Total Energy Considerations

Diffraction experiments cannot determine all structure details.

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Needed: reliable model of the interactions:

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Compromise: use ab-initio derived classical potentials.