INCOMMENSURATE CRYSTAL STRUCTURES

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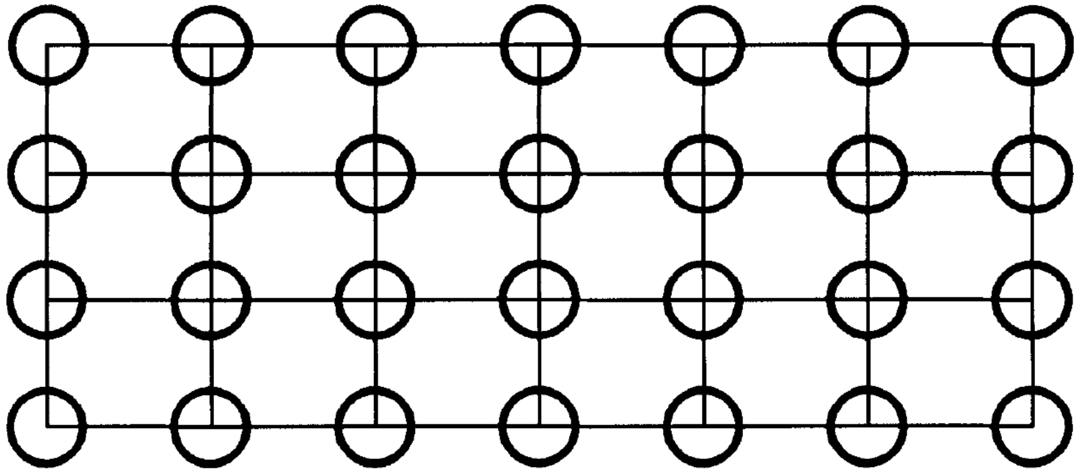
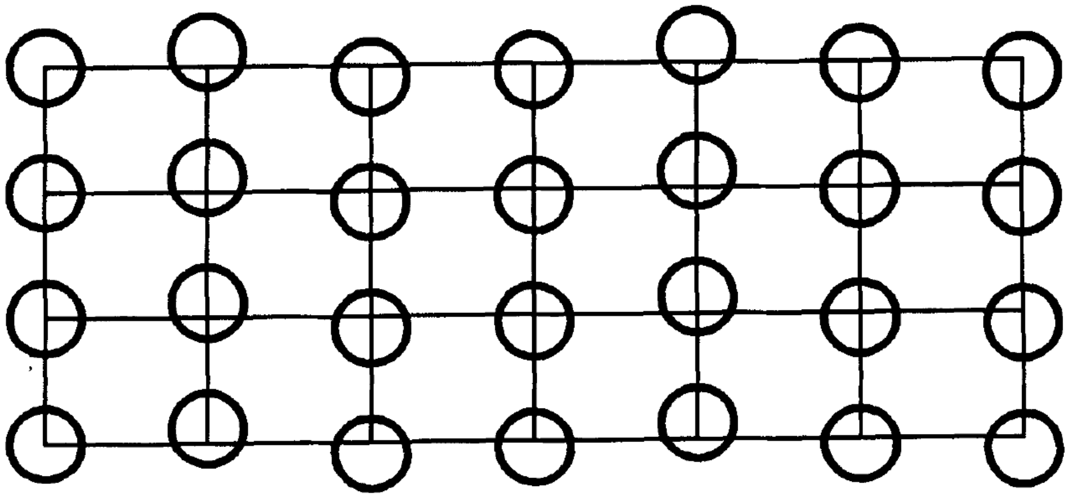
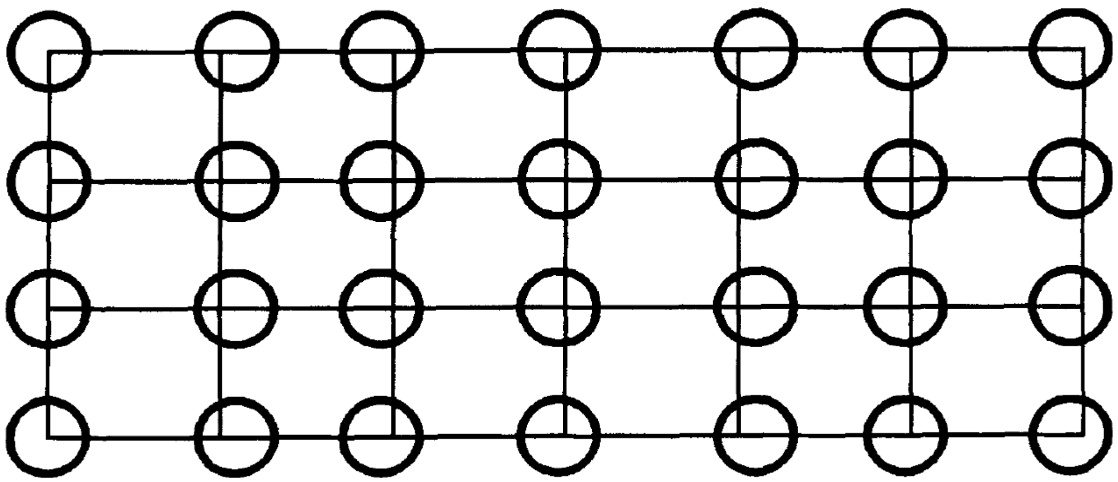
An incommensurately modulated structure



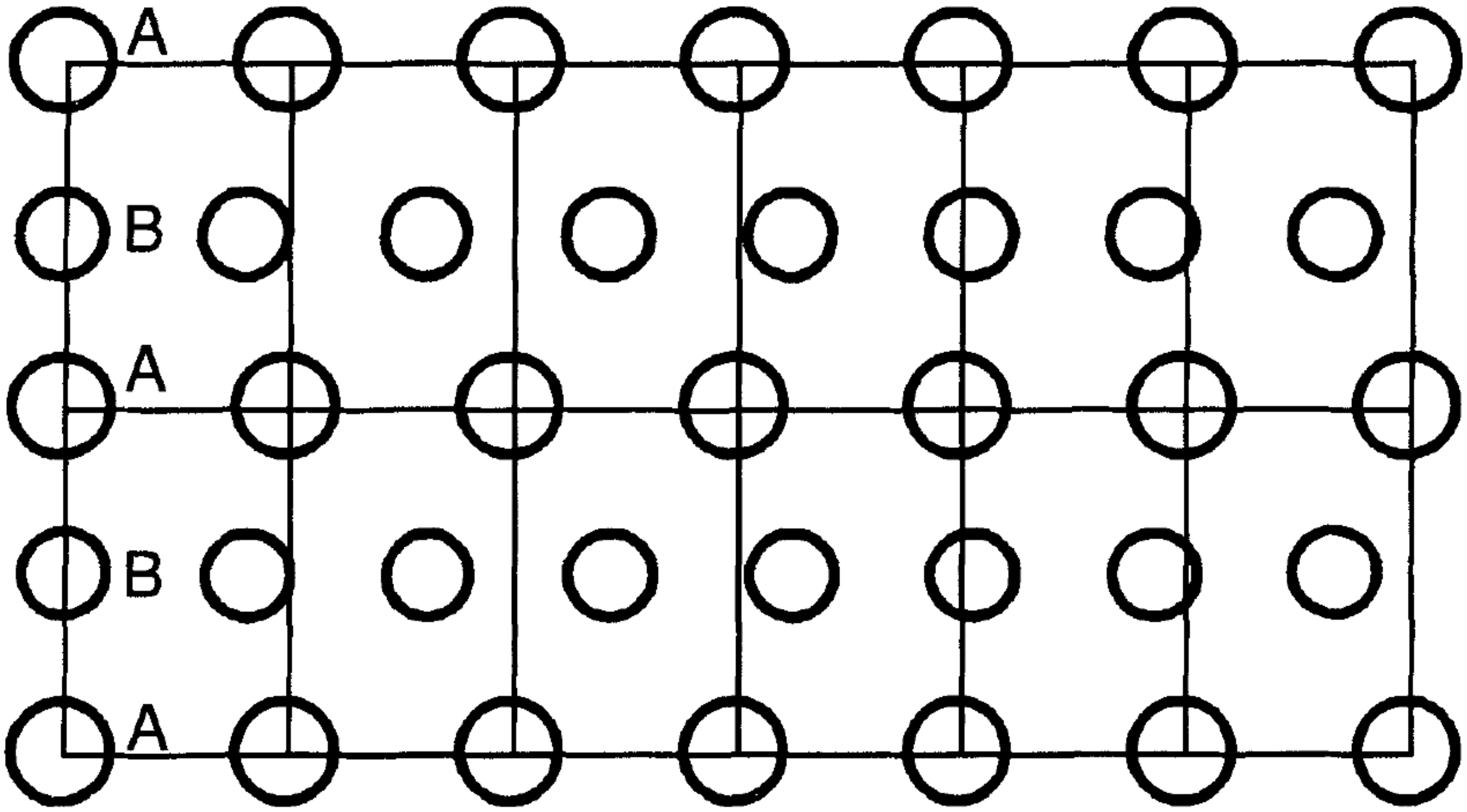
Adding pertrubation





$$u = A\ \sin(2\pi \mathbf{q} \cdot \mathbf{r}) \quad \mathbf{q} = 0.311\ \mathbf{a}^*.$$

Intergrowth compound



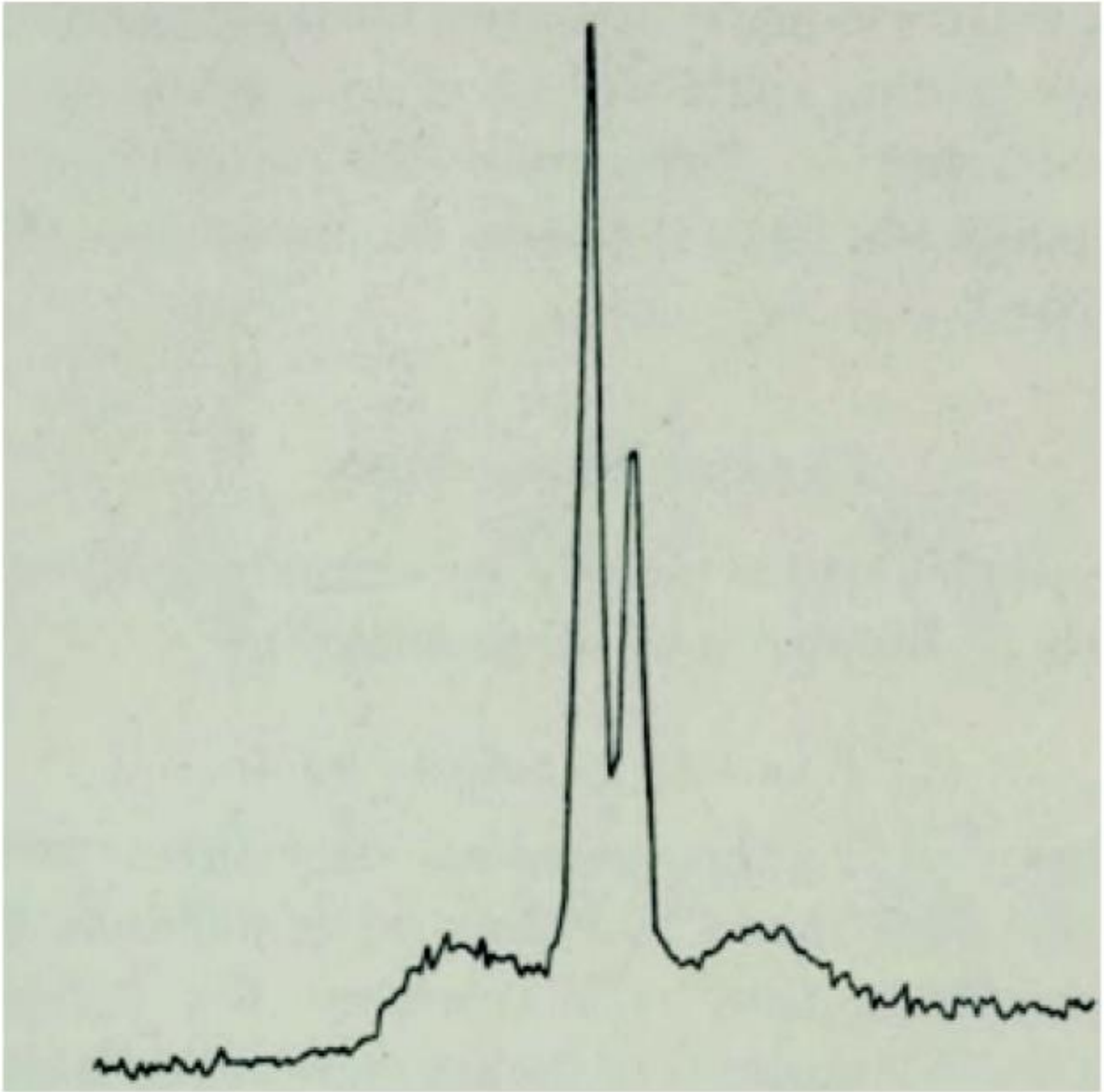
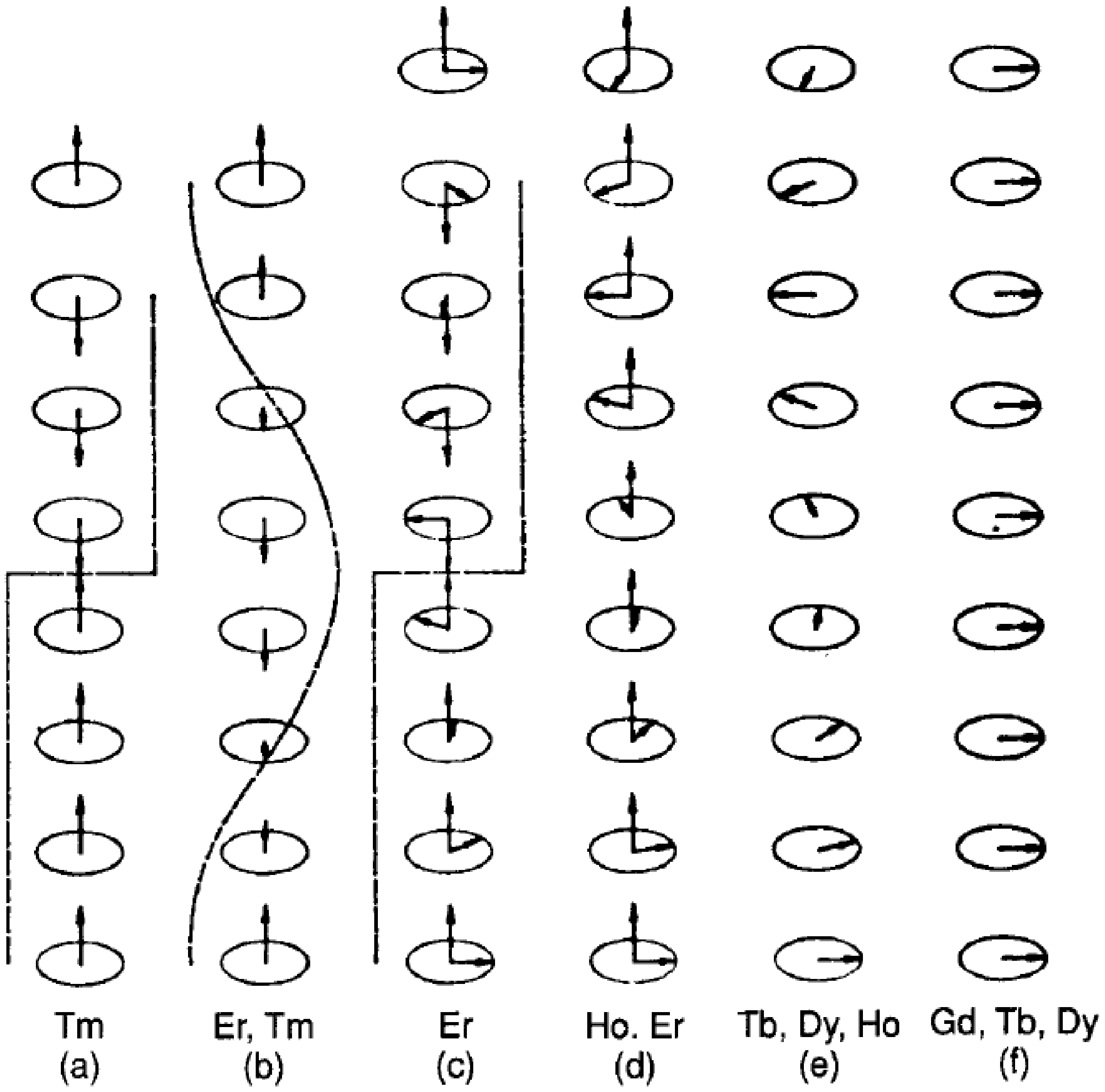


Illustration of one of the first modulated phases observed in a metallic alloy [from Daniel & Lipson (1943)]. The two satellite reflections, a signature of the modulated state, are clear.



Different types of magnetic ordering as observed in the rare earth elements

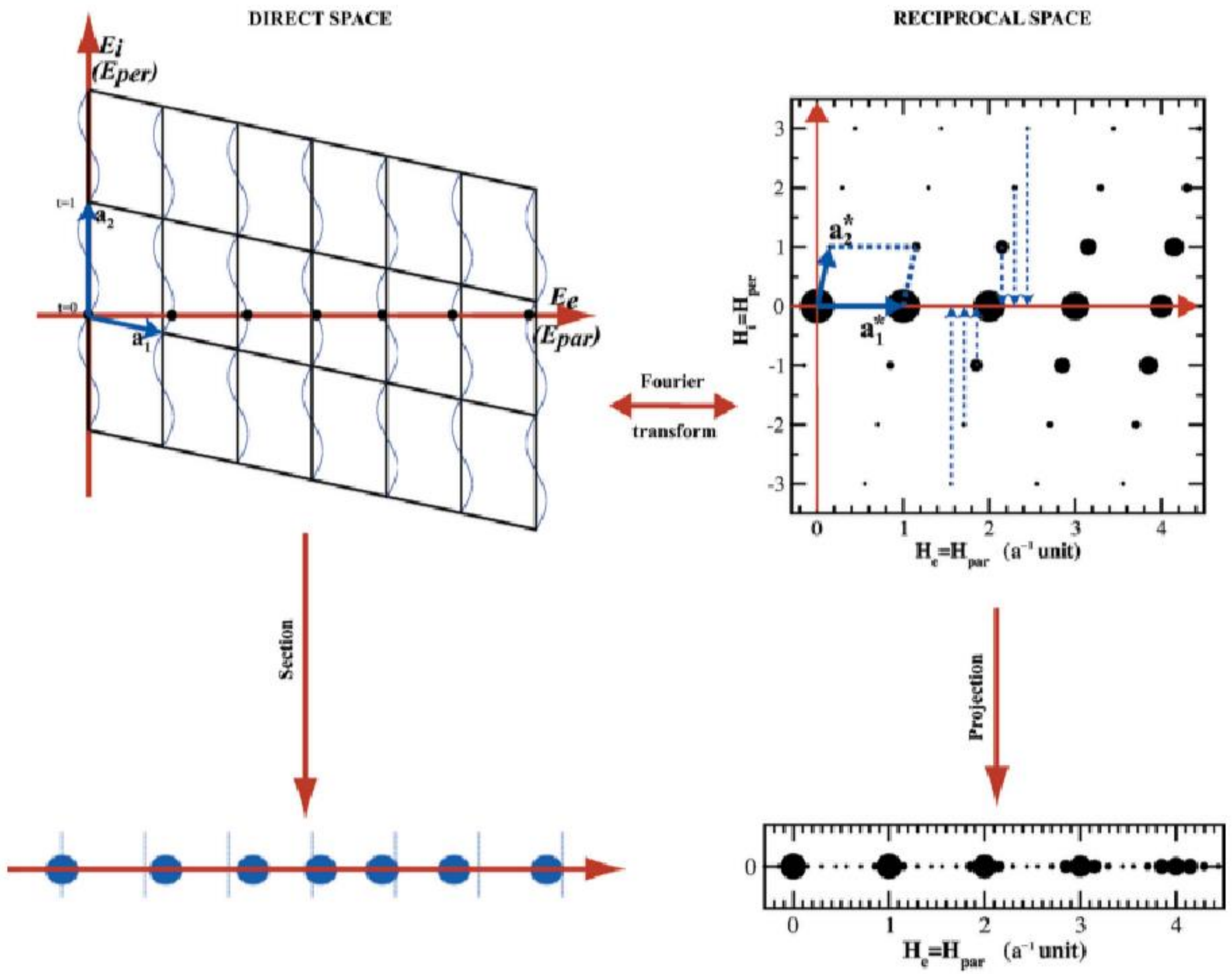
Mathematical description

$$\rho(\mathbf{r}) = \rho_{\Lambda}(\mathbf{r}) + \rho_{\mathbf{k}}(\Lambda;\ \mathbf{r})$$

$$\rho(\mathbf{r}) = \rho_{0}(\mathbf{r}) + \sum_{n=1}^{\infty} A_{n} \cos(2\pi n\mathbf{q} \cdot \mathbf{r}) + B_{n} \sin(2\pi n\mathbf{q} \cdot \mathbf{r})$$

Crystal	$\rho_{\Lambda}(\mathbf{r})$	*point symmetry of the diffraction pattern*
lattice periodic	equal to $\rho(\mathbf{r})$	crystallographic
incommensurately modulated	atom-like for only one lattice	crystallographic
intergrowth	a combination of atom-like and weakly corrugated, for each of the N lattices corresponding to the N subsystems	crystallographic
quasicrystal	as intergrowth	non-crystallographic

Example of superspace crystallography in the case of a 1D incommensurately modulated phase



(i) *First step.* Determine the Laue group of the diffraction pattern.

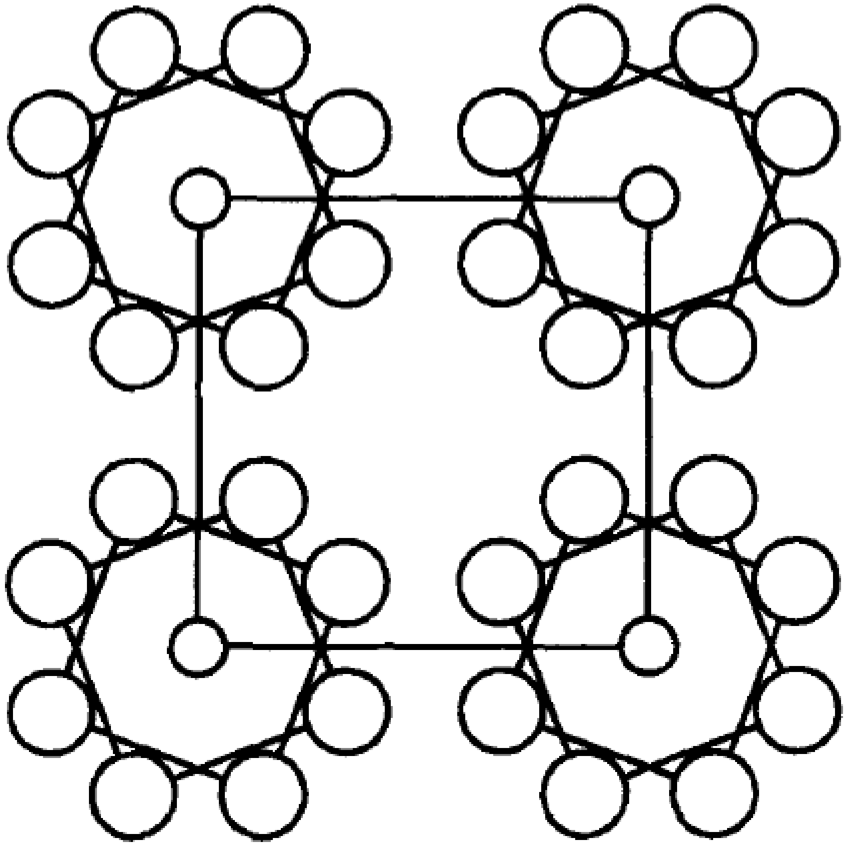
(ii) *Second step.* Choose a basis for the basic structure according to *International Tables for Crystallography* (Vol. A), and extend its reciprocal basis to a basis of the Fourier module.

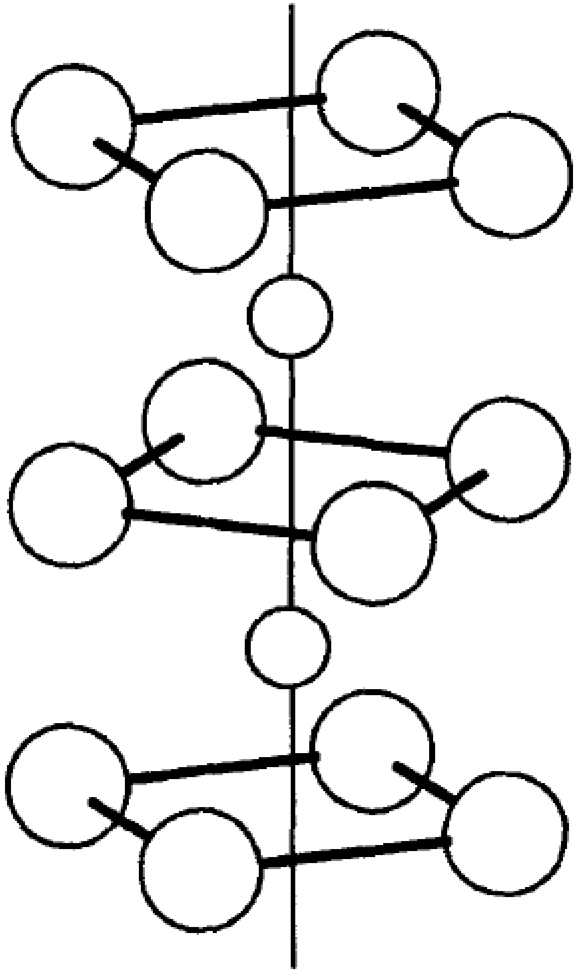
(iii) *Third step.* Determine the space group of the average structure, obtained from the main reflections.

(iv) *Fourth step.* Determine the Bravais lattice type in superspace, using the observed extinctions. This also implies the choice of a conventional cell.

(v) *Fifth step.* Determine the possible superspace groups associated with the space group of the basic structure are compatible with the observed extinctions.

$NbTe_4$



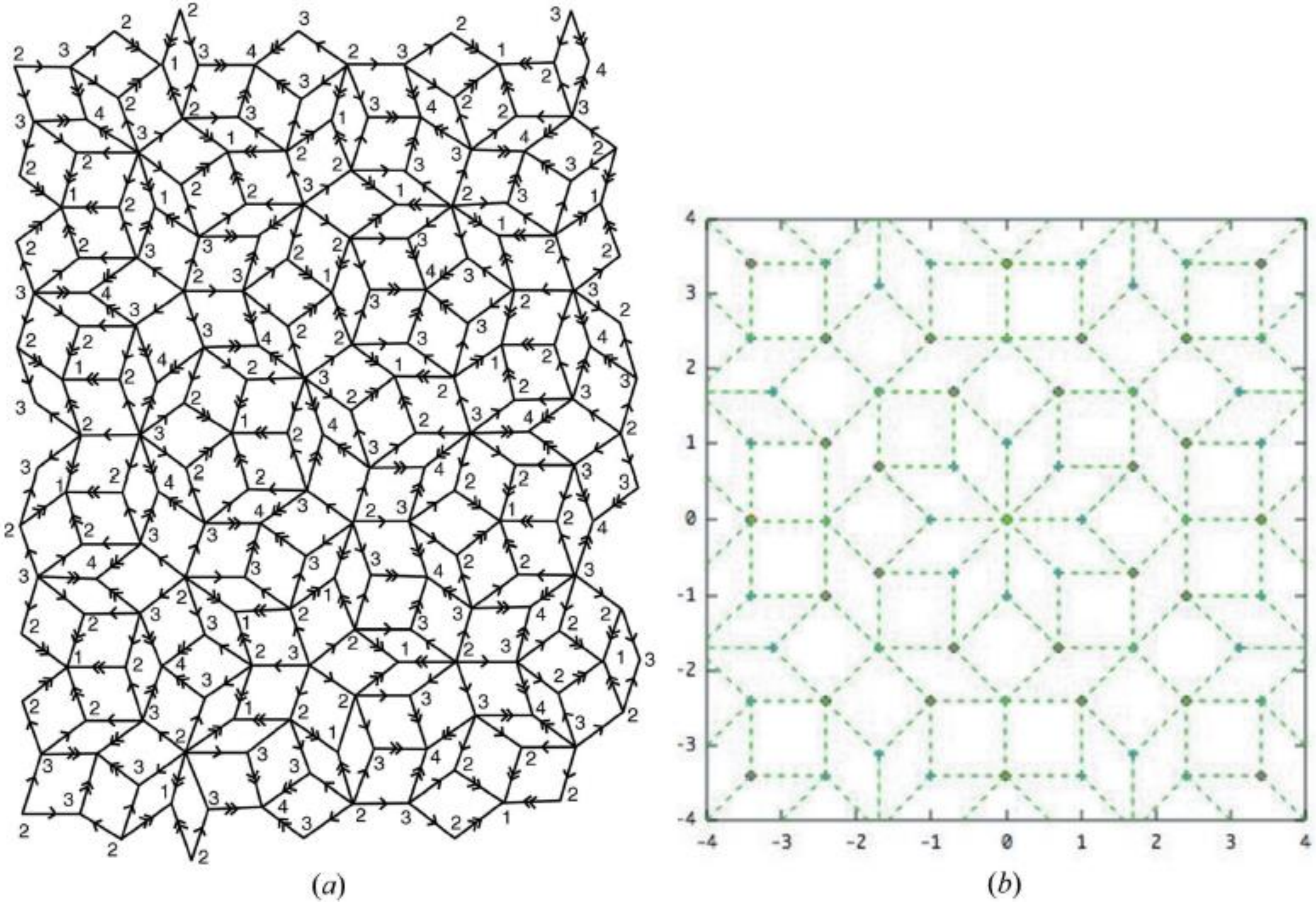


For room temperature: $a = b = 6.499$ Å and $c = 6.837$ Å $\mathbf{q} = (1/2, 1/2, 0.691)$

Above 793K no modulation

Low temperatures: commensurate with a $2a \times 2a \times 3c$ supercell

Quasicrystals



(a) An example of a Penrose tiling. (b) The Ammann–Beenker tiling.

Sources:

[1] Sander Van Smaalen (1995): Incommensurate crystal structures, Crystallography Reviews, 4:2, 79-202
[2] W. C. Koehler, Magnetic Properties of Rare Earth Metals, 1972
[3] Marc de Boissieu, Ted Janssen and aperiodic crystals, Acta Crystallographica Section A: Foundations and Advances 75(2), 2019
[4] T. Janssen and A. Janner, Aperiodic crystals and superspace concepts, Acta Crystallographica Section B, 2014
[5] Заметки к лекциям по общей физике, В.Н. Глазков