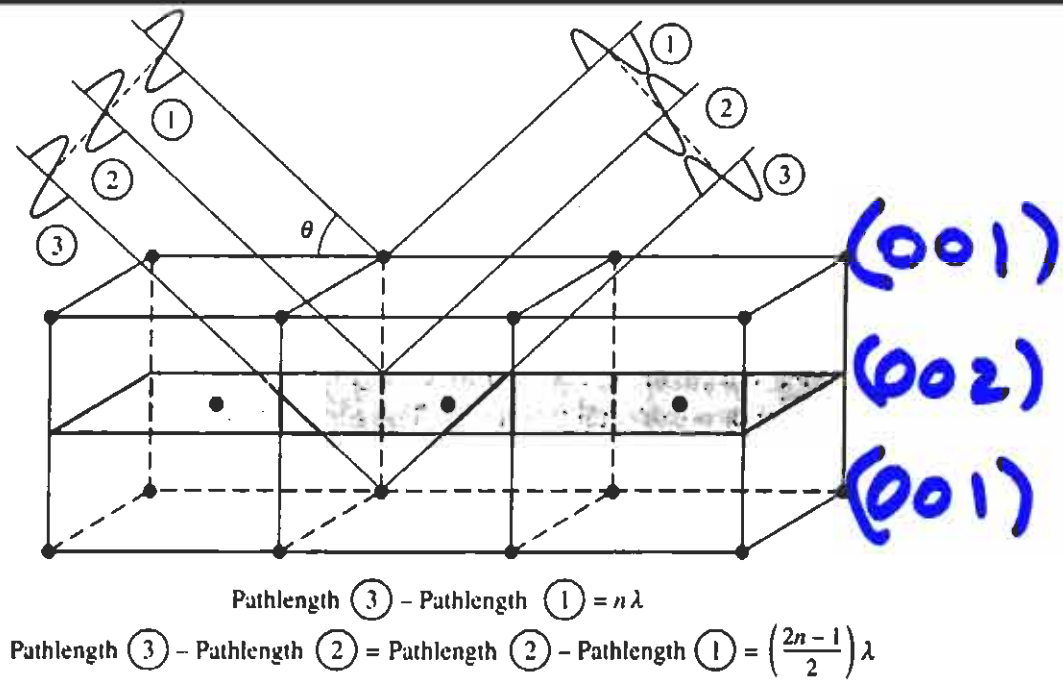
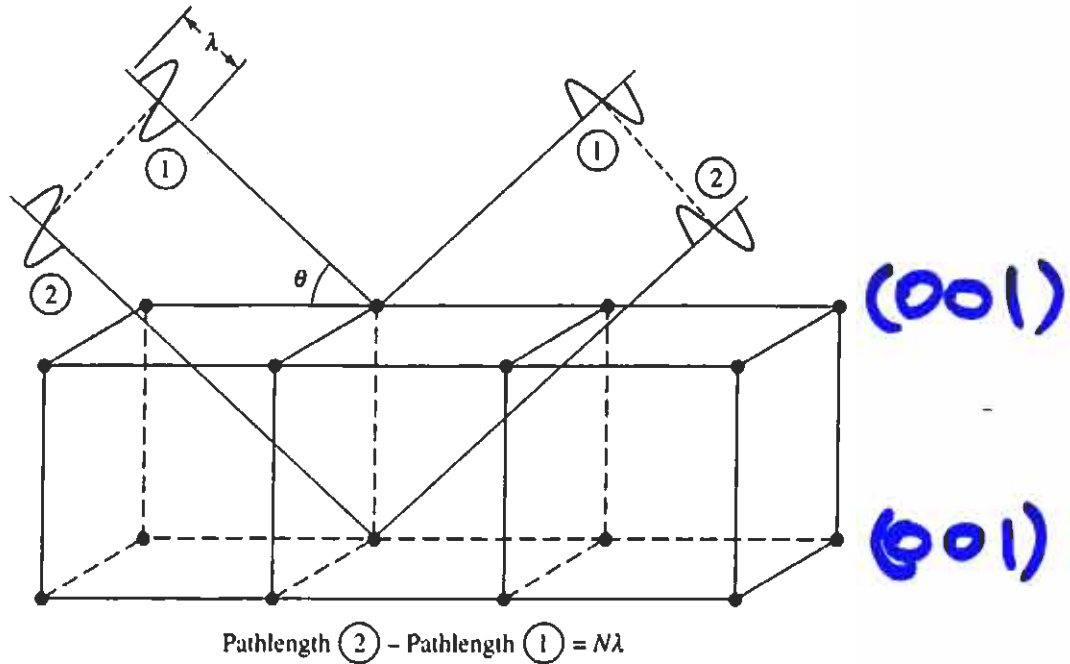


Welcome to 3.091

Lecture 18

October 22, 2004



Selection Rules for Reflection in Cubic Crystals

(hkl)	$h^2+k^2+l^2$	SC	BCC	FCC
100	1	✓	✗	✗
110	2	✓	✓	✗
111	3	✓	✗	✓
200	4	✓	✓	✓
210	5	✓	✗	✗
211	6	✓	✓	✗
220	8	✓	✓	✓
300	9	✓	✗	✗
310	10	✓	✓	✗
311	11	✓	✗	✓
222	12	✓	✓	✓
320	13	✓	✗	✗
321	14	✓	✓	✗
400	16	✓	✓	✓

Selection Rules for Reflection in Cubic Crystals

(hkl)	$h^2+k^2+l^2$	SC	BCC	FCC
100	1	✓	✗	✗
110	2	✓	✓	✗
111	3	✓	✗	✓
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210	5	✓	✗	✗
211	6	✓	✓	✗
220	8	✓	✓	✗
300	9	✓	✗	✗
310	10	✓	✓	✗
311	11	✓	✗	✓
222	12	✓	✓	✓
320	13	✓	✗	✗
321	14	✓	✓	✗
400	16	✓	✓	✓

all

*h+k+l
even*

*h, k, l
all even
or
all odd
"unmixed"*

Cu target, $\lambda_{K\alpha} = 1.5418 \text{ \AA}$

2 θ

44.48

51.83

76.35

92.90

98.40

121.87

144.54

155.51

Sadoway's Five-step Program for Determining Crystal Structure

Step 1 Start with 2θ values and generate a set of $\sin^2\theta$ values.

Cu target, $\lambda_{K\alpha} = 1.5418 \text{ \AA}$

2θ	$\sin^2 \theta$
44.48	0.143
51.83	0.191
76.35	0.382
92.90	0.525
98.40	0.573
121.87	0.764
144.54	0.907
155.51	0.955

Sadoway's Five-step Program for Determining Crystal Structure

- Step 1** Start with 2θ values and generate a set of $\sin^2\theta$ values.
- Step 2** Normalize the $\sin^2\theta$ values by generating $\sin^2\theta_n / \sin^2\theta_1$.

Cu target, $\lambda_{K\alpha} = 1.5418 \text{ \AA}$

2θ	$\sin^2 \theta$	
44.48	0.143	1.00
51.83	0.191	1.34
76.35	0.382	2.67
92.90	0.525	3.67
98.40	0.573	4.01
121.87	0.764	5.34
144.54	0.907	6.34
155.51	0.955	6.68

Sadoway's Five-step Program for Determining Crystal Structure

- Step 1** Start with 2θ values and generate a set of $\sin^2\theta$ values.
- Step 2** Normalize the $\sin^2\theta$ values by generating $\sin^2\theta_n / \sin^2\theta_1$.
- Step 3** Clear fractions from “normalized” column.

Cu target, $\lambda_{K\alpha} = 1.5418 \text{ \AA}$

2θ	$\sin^2 \theta$	normalized	clear
			fractions
44.48	0.143	1.00	3
51.83	0.191	1.34	4
76.35	0.382	2.67	8
92.90	0.525	3.67	11
98.40	0.573	4.01	12
121.87	0.764	5.34	16
144.54	0.907	6.34	19
155.51	0.955	6.68	20

Sadoway's Five-step Program for Determining Crystal Structure

- Step 1** Start with 2θ values and generate a set of $\sin^2\theta$ values.
- Step 2** Normalize the $\sin^2\theta$ values by generating $\sin^2\theta_n / \sin^2\theta_1$.
- Step 3** Clear fractions from “normalized” column.
- Step 4** Speculate on the hkl values that, if expressed as $h^2+k^2+l^2$, would generate the sequence of the “clear fractions” column.

Cu target, $\lambda_{K\alpha} = 1.5418 \text{ \AA}$

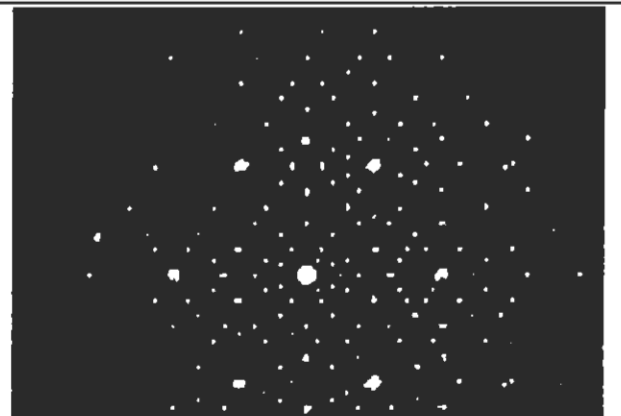
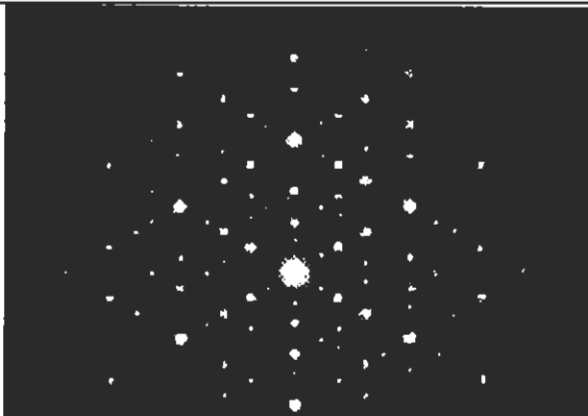
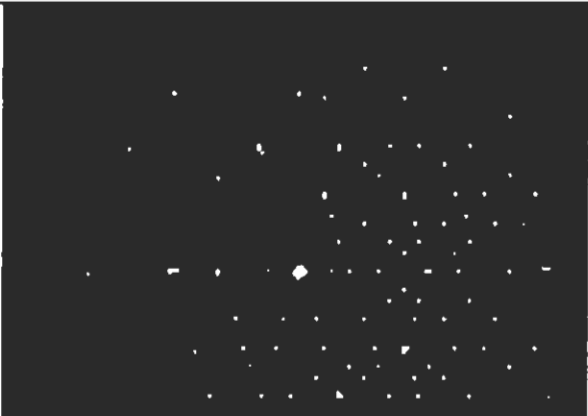
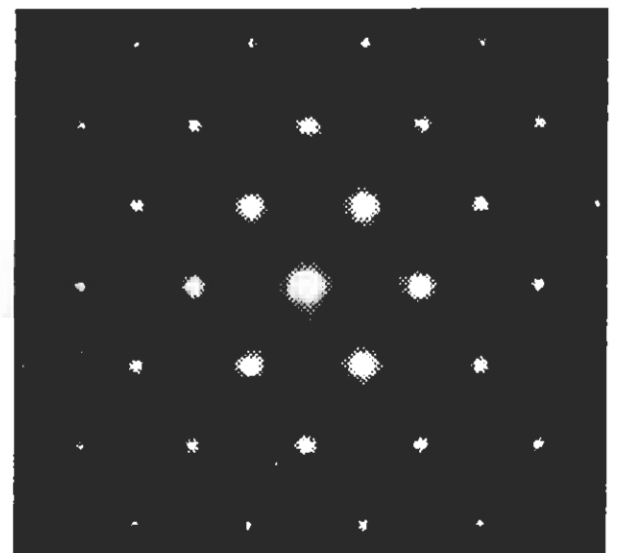
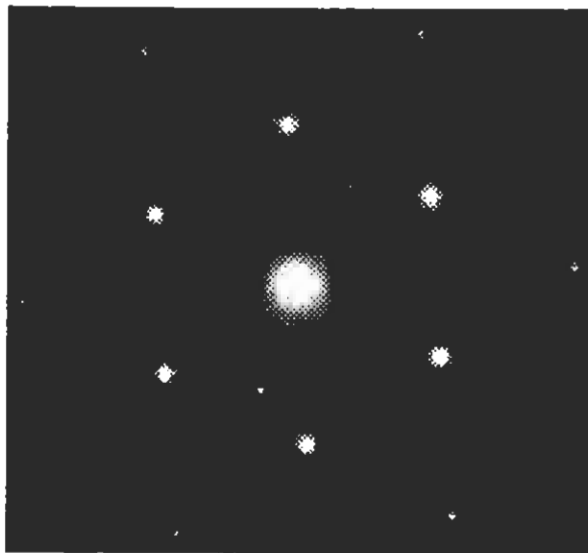
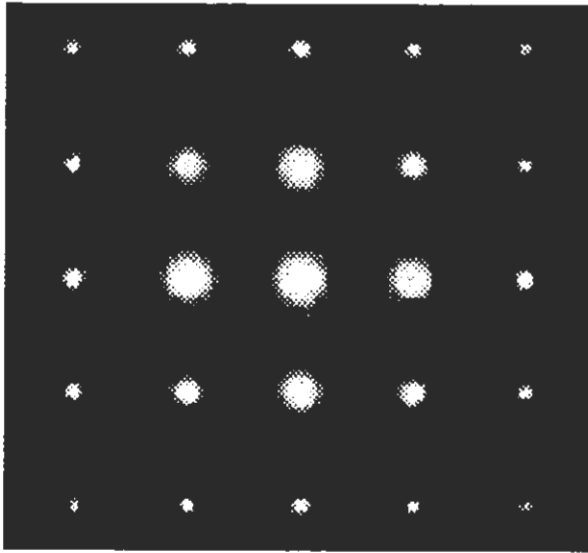
2θ	$\sin^2 \theta$	normalized	clear	(hkl)?
			fractions	
44.48	0.143	1.00	3	111
51.83	0.191	1.34	4	200
76.35	0.382	2.67	8	220
92.90	0.525	3.67	11	311
98.40	0.573	4.01	12	222
121.87	0.764	5.34	16	400
144.54	0.907	6.34	19	331
155.51	0.955	6.68	20	420

Sadoway's Five-step Program for Determining Crystal Structure

- Step 1** Start with 2θ values and generate a set of $\sin^2\theta$ values.
- Step 2** Normalize the $\sin^2\theta$ values by generating $\sin^2\theta_n / \sin^2\theta_1$.
- Step 3** Clear fractions from “normalized” column.
- Step 4** Speculate on the hkl values that, if expressed as $h^2+k^2+l^2$, would generate the sequence of the “clear fractions” column.
- Step 5** Compute for each θ the value of $\sin^2\theta / (h^2+k^2+l^2)$ on the basis of the assumed hkl values. If each entry in this column is identical, then the entire process is validated.

Cu target, $\lambda_{K\alpha} = 1.5418 \text{ \AA}$

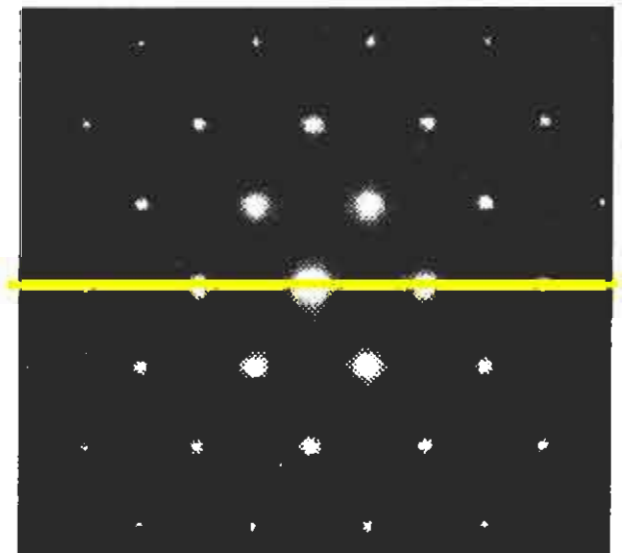
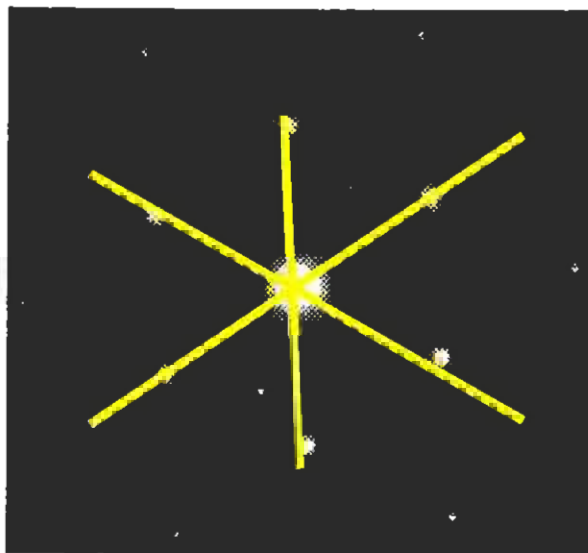
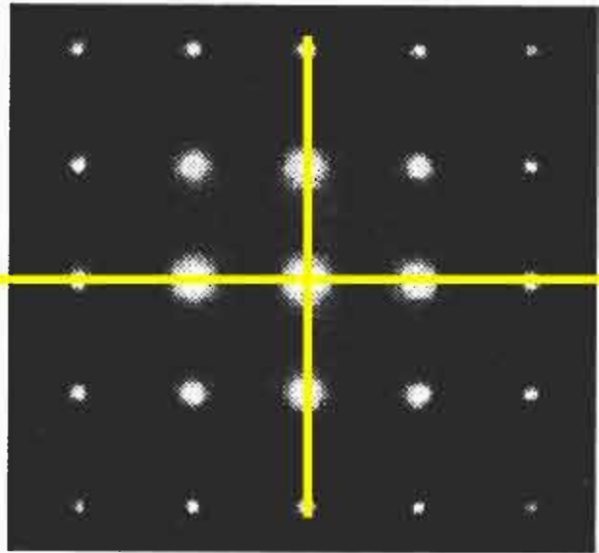
2θ	$\sin^2 \theta$	normalized	clear	(hkl)?	$\frac{\sin^2 \theta}{h^2 + k^2 + l^2}$
		fractions			
44.48	0.143	1.00	3	111	0.0477
51.83	0.191	1.34	4	200	0.0478
76.35	0.382	2.67	8	220	0.0478
92.90	0.525	3.67	11	311	0.0477
98.40	0.573	4.01	12	222	0.0478
121.87	0.764	5.34	16	400	0.0477
144.54	0.907	6.34	19	331	0.0477
155.51	0.955	6.68	20	420	0.0478



4-fold

3-fold

2-fold

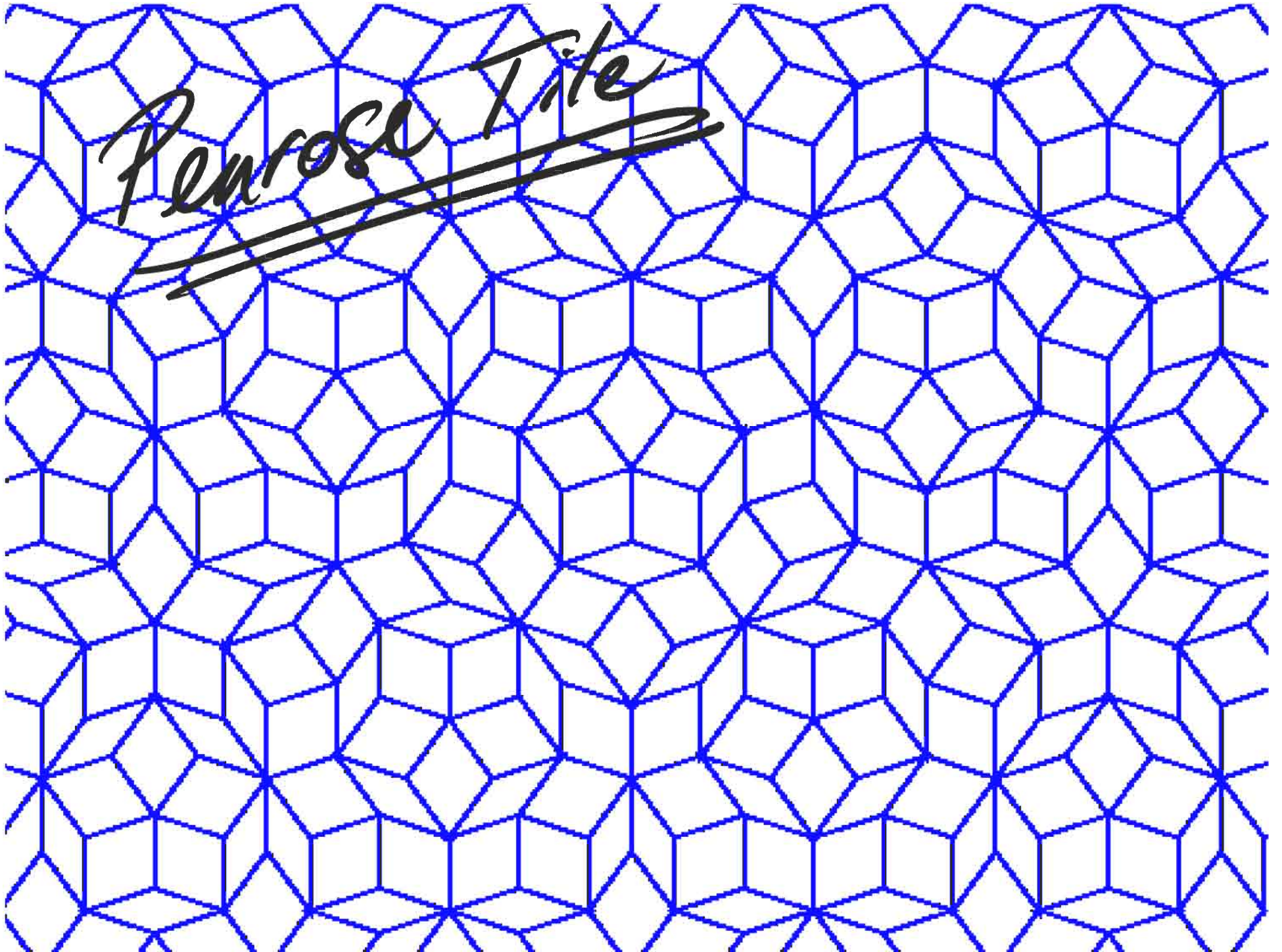


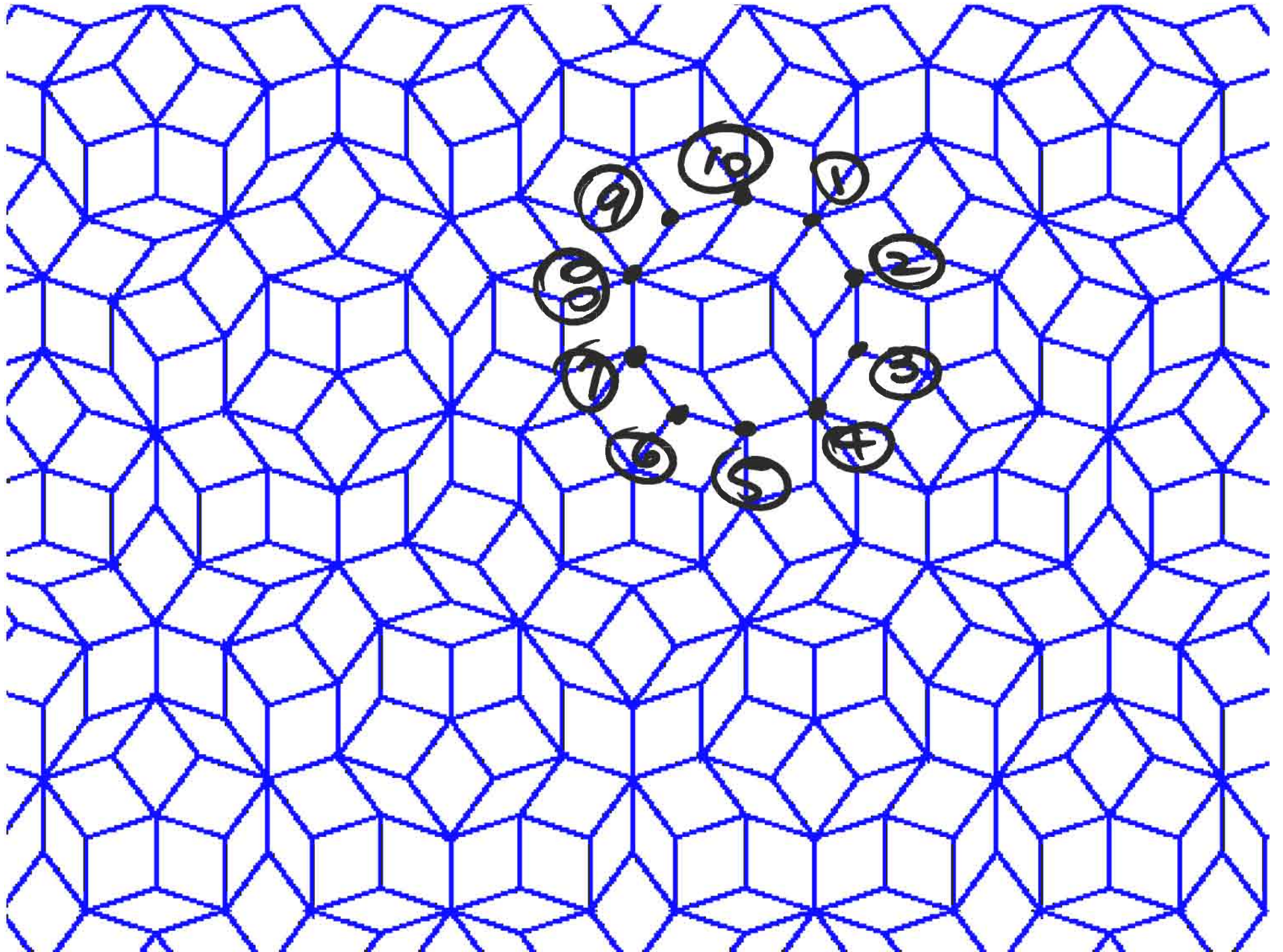
90°

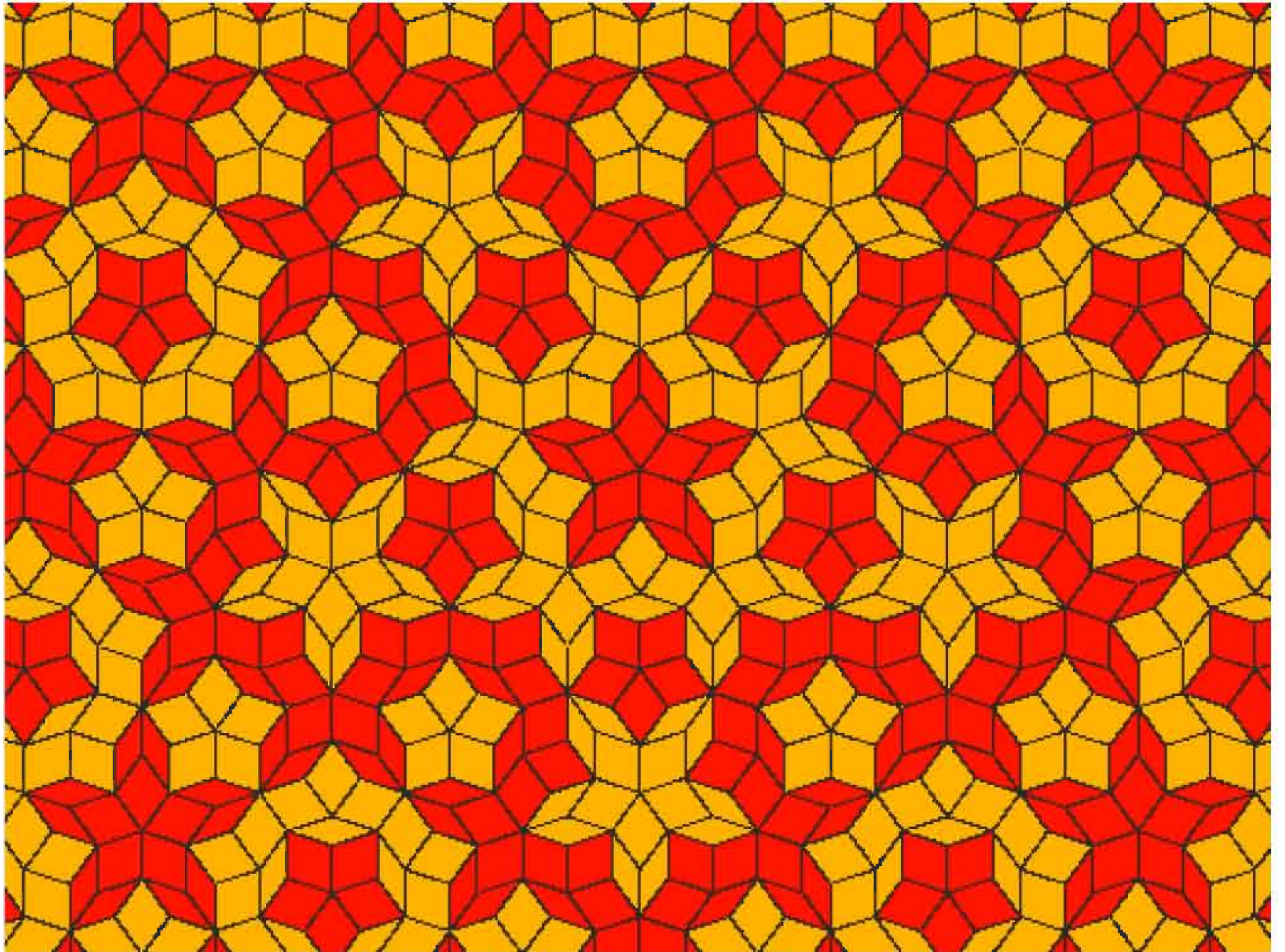
120°

180°

Penrose Tile







Taxonomy of Solids

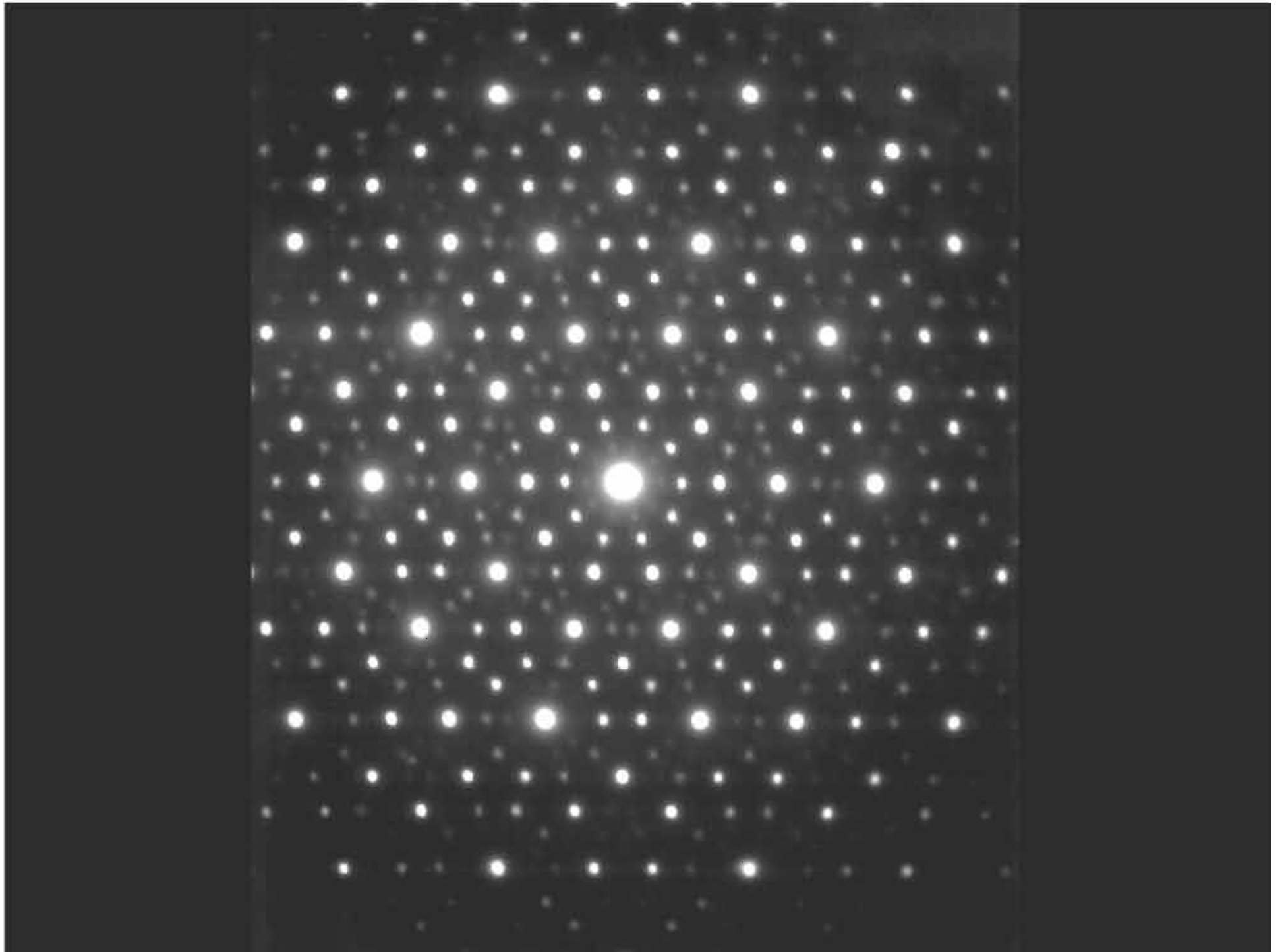
- | ordered | disordered |
|-------------|-----------------------|
| - unit cell | - no building block |
| - periodic | - no long-range order |
| - “crystal” | - “glass” |

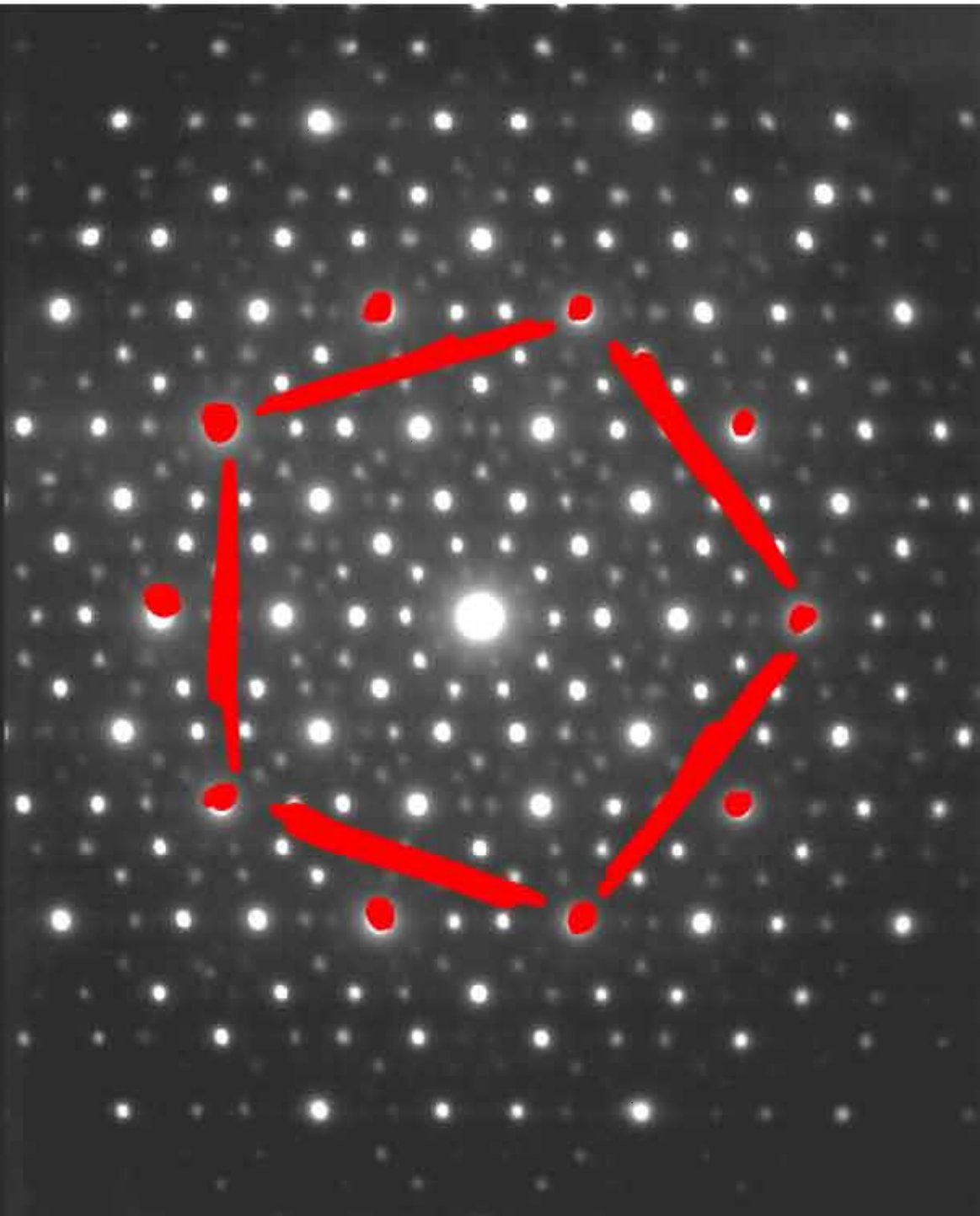
1982 Dan Schechtman (Technion) working at National Institute of Standards and Technology (NIST), Gaithersburg, MD

Al - Mn alloy:

- highly ordered
- symmetries impossible in a true crystal (5-fold rotational symmetry)
- lacks translational symmetry: *aperiodic*

“quasicrystals”





5-fold

72°

