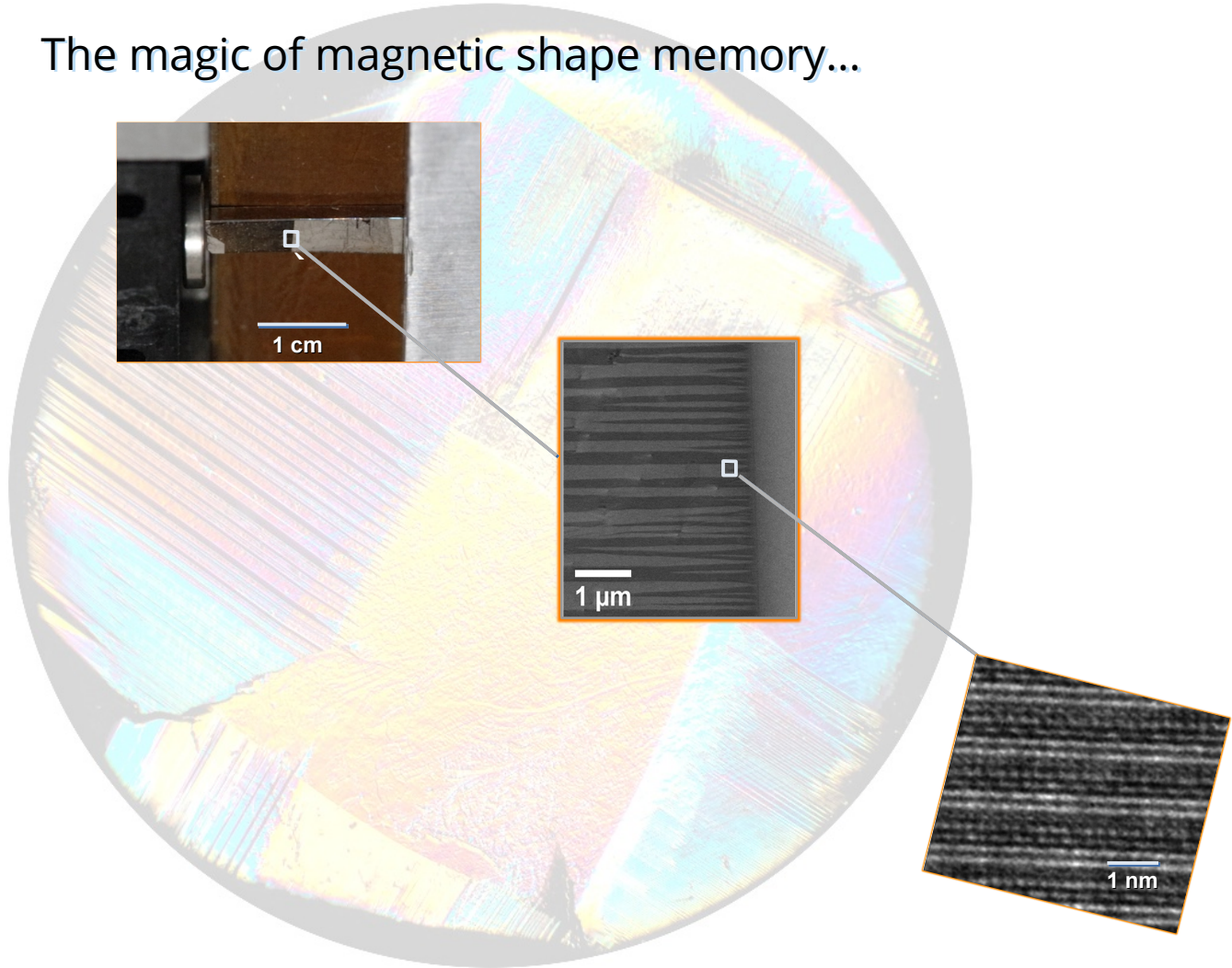
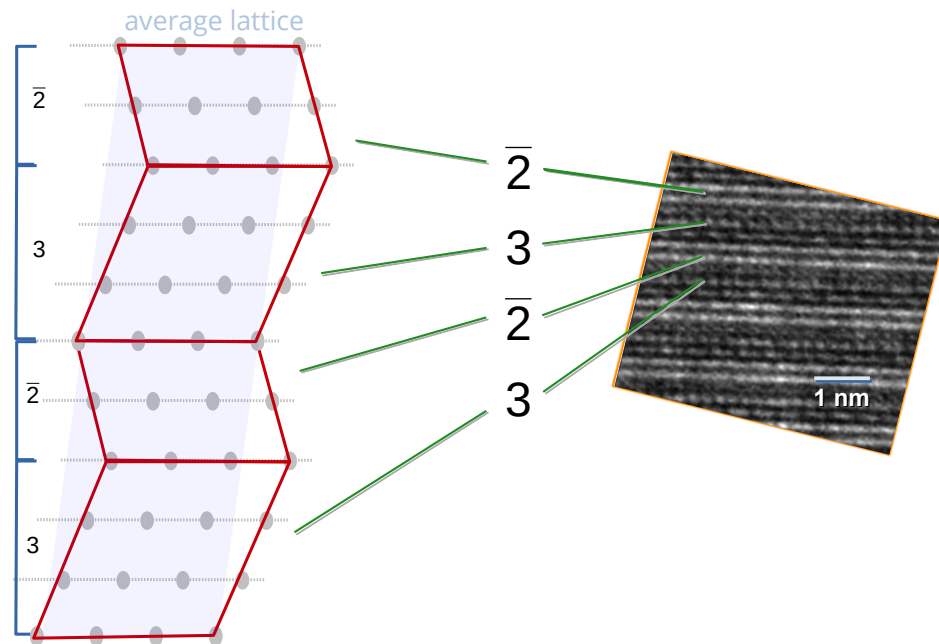


The magic of magnetic shape memory...

- Intro & macrotwins
- *Movie with examples*
- Microtwins
- Nanotwins
- Summary

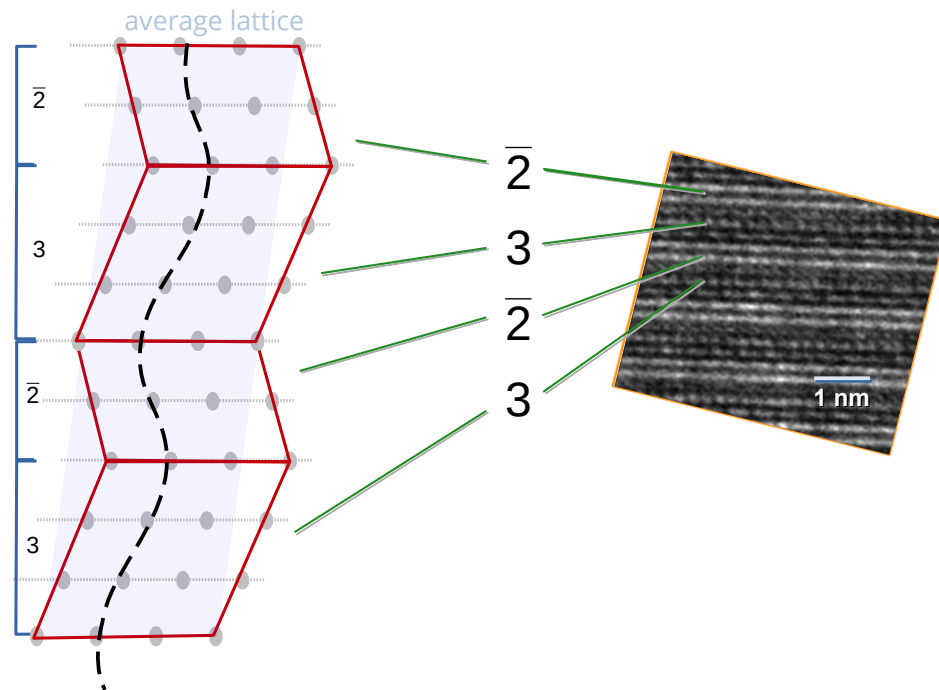


Structure as a $3\bar{2}$ stacking sequence



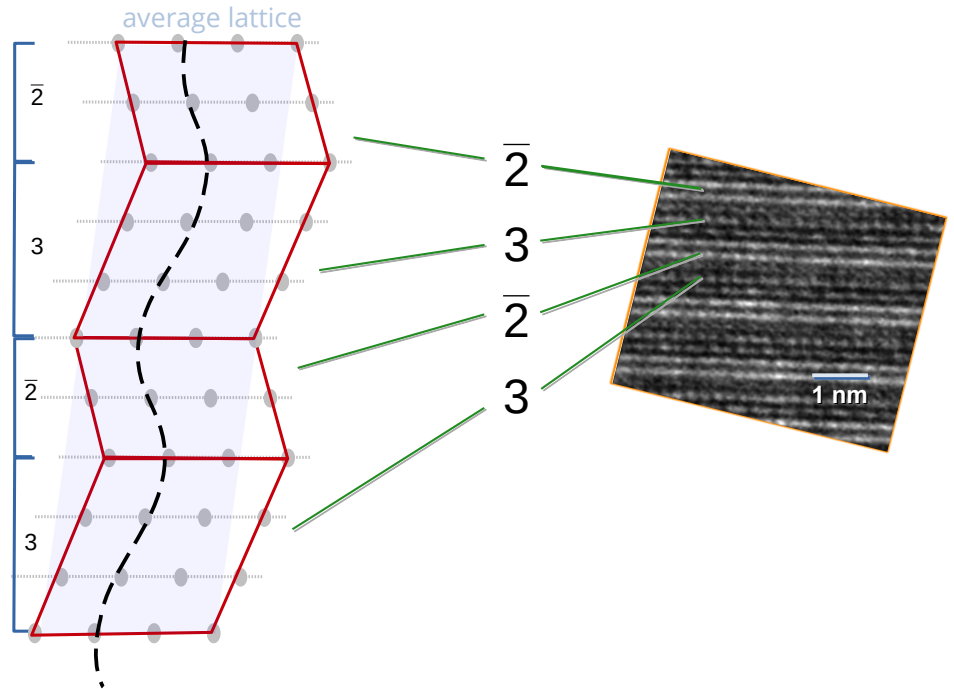
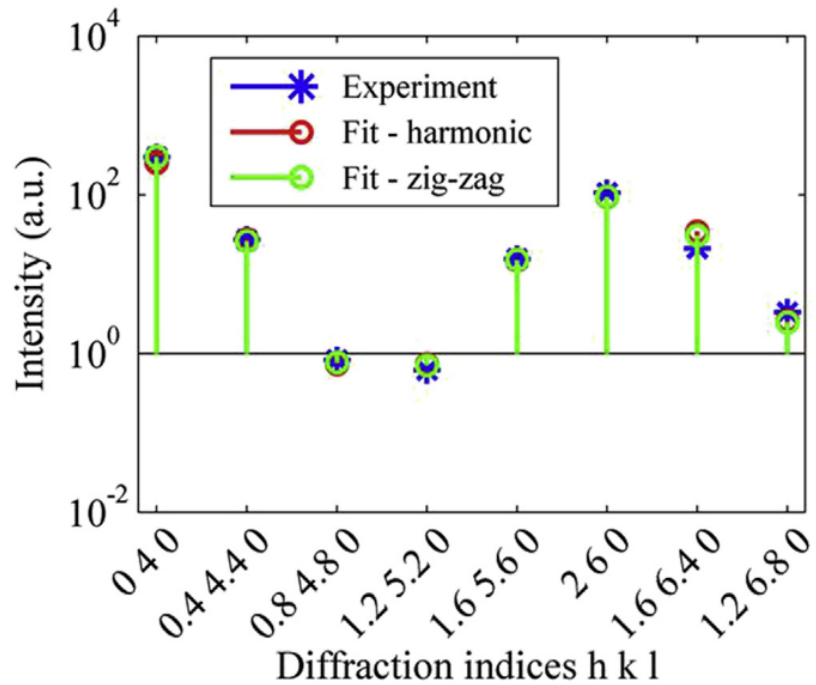
Straka, L., et al., Acta Materialia 132 (2017): 335-344.
 Straka, L., et al., Scientific Reports 8.1 (2018): 11943.

Structure as a $3\bar{2}$ stacking sequence



Straka, L., et al., Acta Materialia 132 (2017): 335-344.
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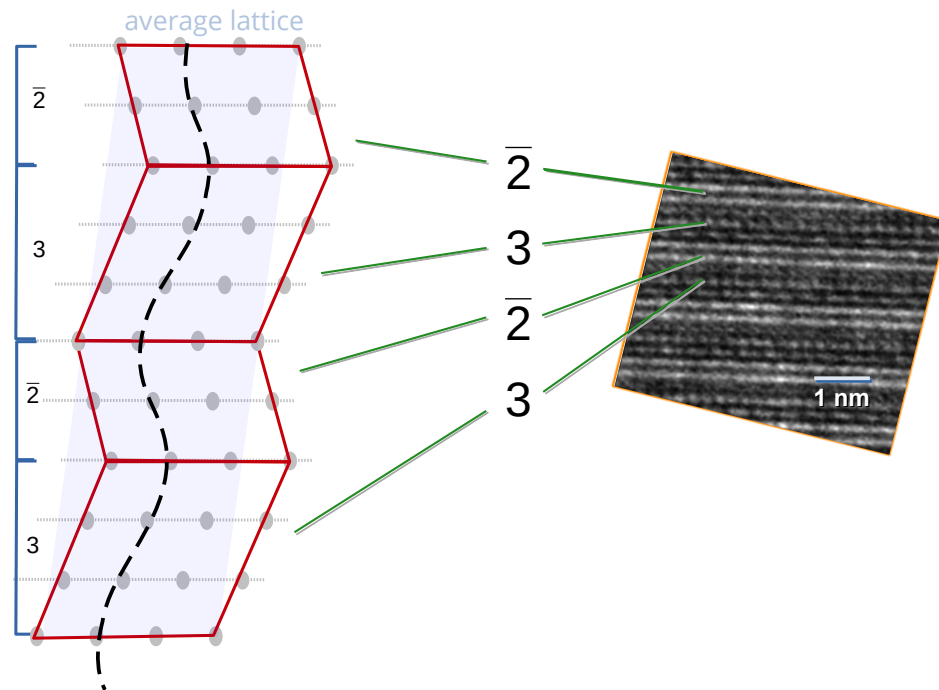
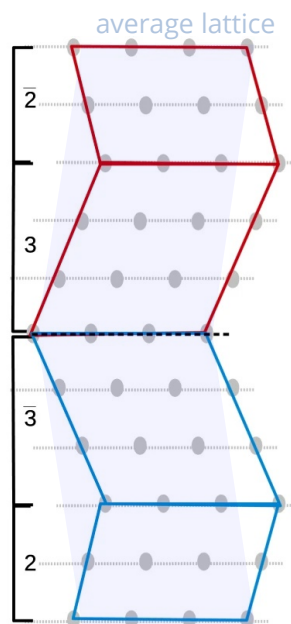
Structure as a $3\bar{2}$ stacking sequence



Heczko, Oleg, et al. Acta Materialia 115 (2016): 250-258.

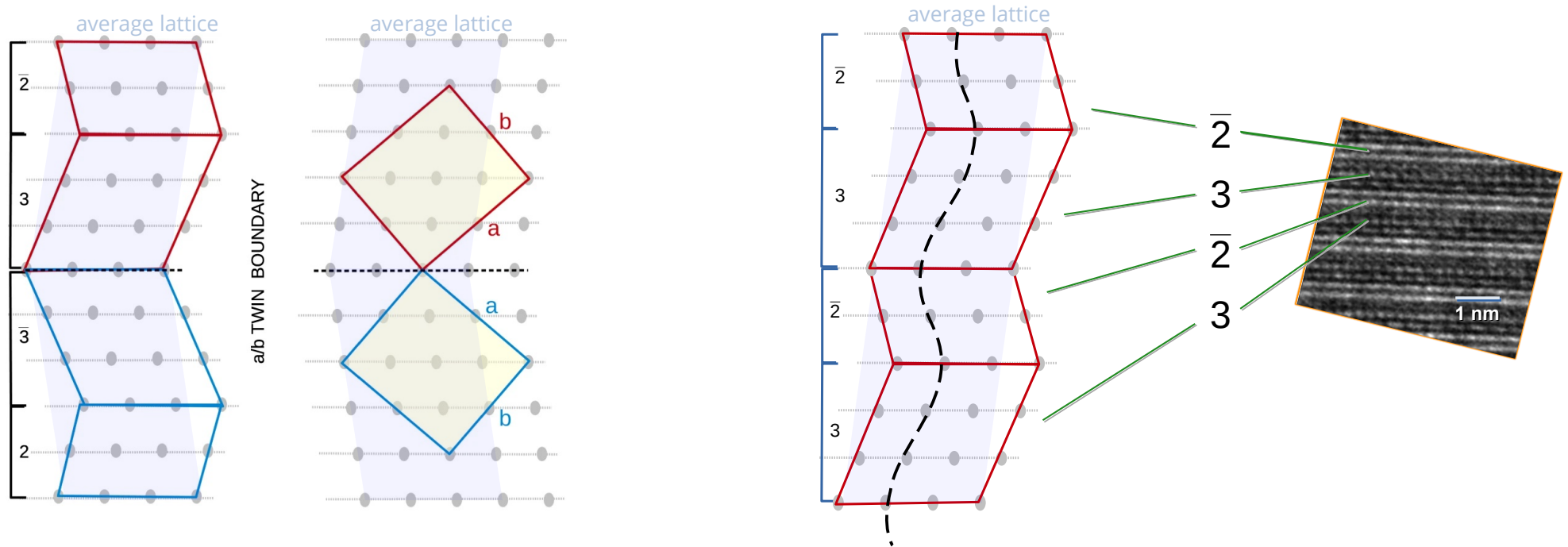
Straka, L., et al., Acta Materialia 132 (2017): 335-344.
Straka, L., et al., Scientific Reports 8.1 (2018): 11943.

Structure as a $3\bar{2}$ stacking sequence



Straka, L., et al., Acta Materialia 132 (2017): 335-344.
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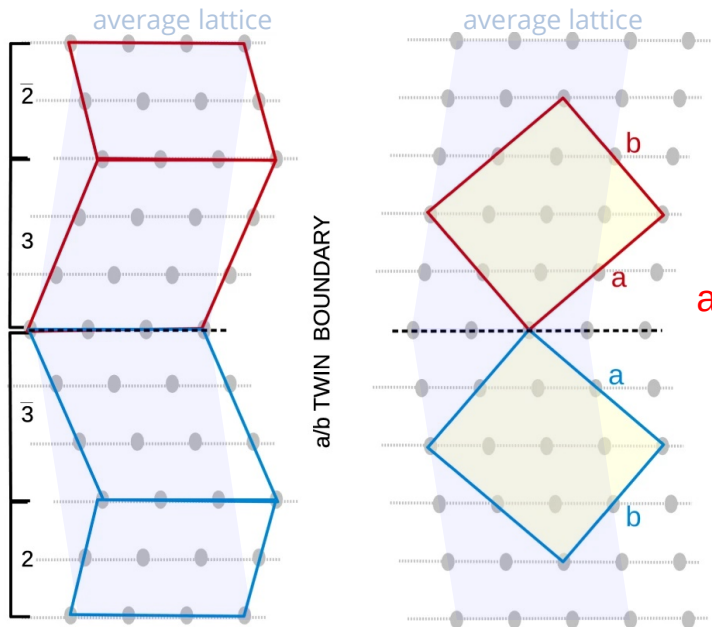
Structure as a $3\bar{2}$ stacking sequence



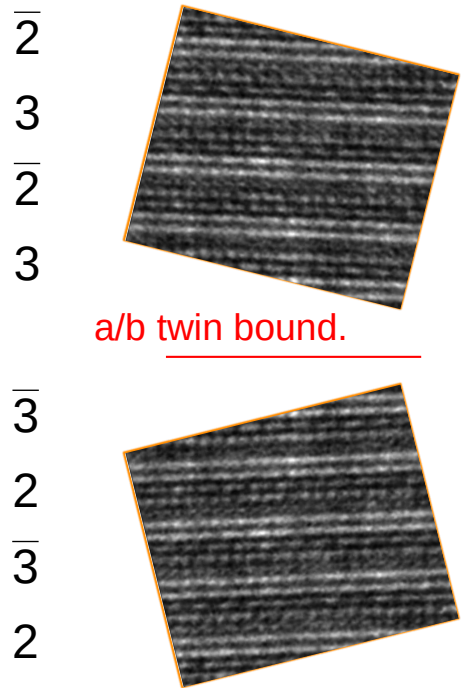
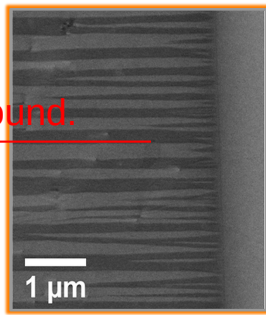
Straka, L., et al., Acta Materialia 132 (2017): 335-344.
 Straka, L., et al., Scientific Reports 8.1 (2018): 11943.

a/b twins as a $\overline{3}\overline{2}$ stacking sequence inversion

a/b twin boundary = stacking sequence inversion ... $\overline{3}\overline{2}\overline{3}\overline{2}\overline{3}\overline{2}$ | $\overline{2}\overline{3}\overline{2}\overline{3}\overline{2}$...



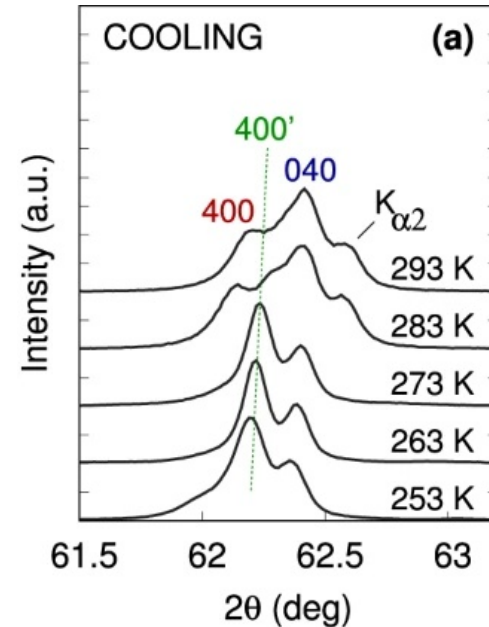
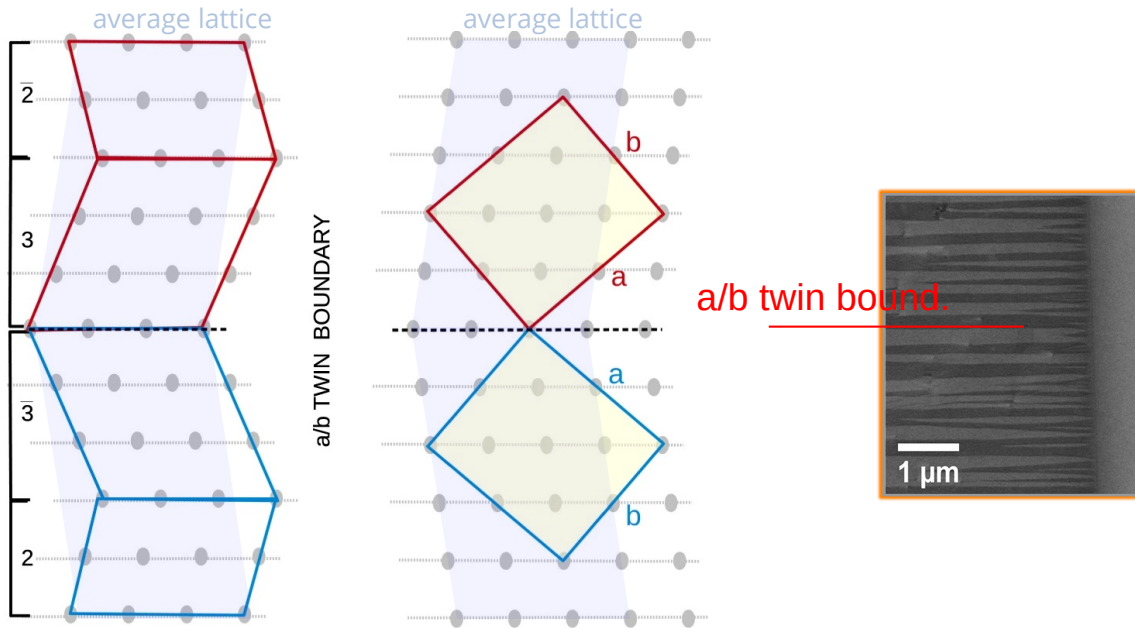
a/b twin bound.



Straka, L., et al., Acta Materialia 132 (2017): 335-344.
Straka, L., et al., Scientific Reports 8.1 (2018): 11943.

a/b twins as a $3\bar{2}$ stacking sequence inversion

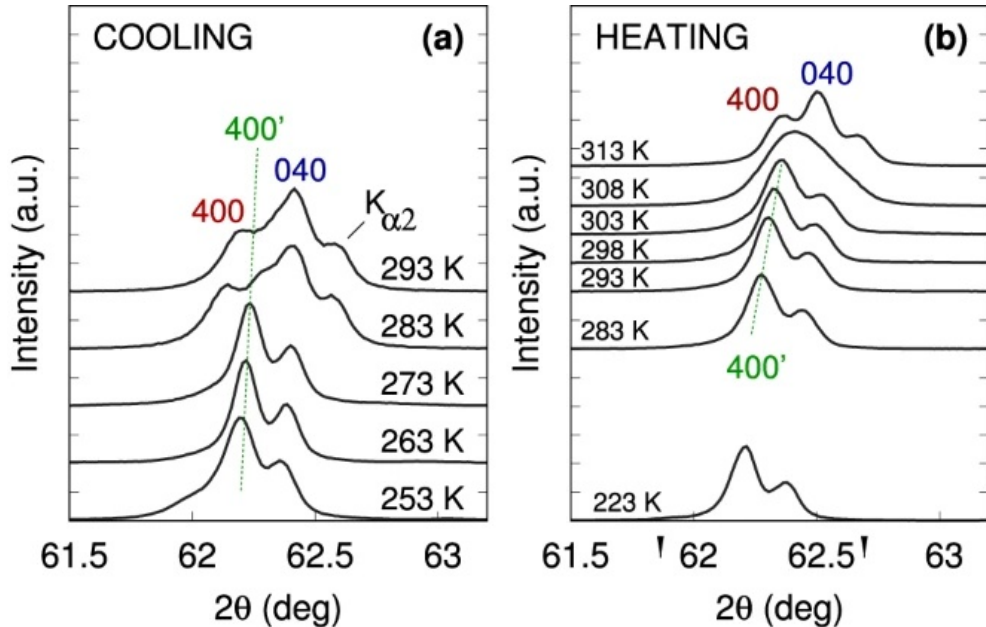
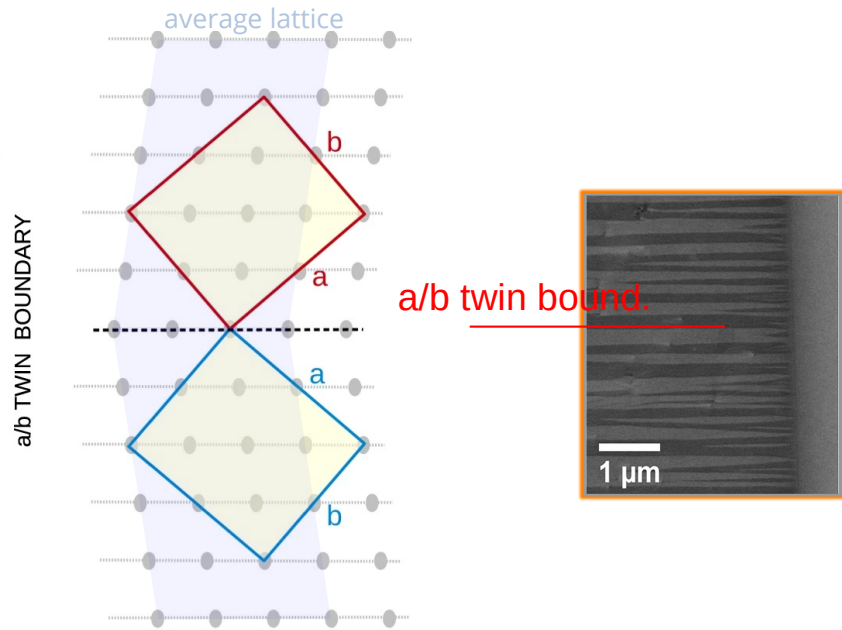
a/b twin boundary = stacking sequence inversion ... $3\bar{2}3\bar{2}3\bar{2}$ | $2\bar{3}2\bar{3}2\bar{3}$...



Straka, L., et al., Acta Materialia 132 (2017): 335-344.
 Straka, L., et al., Scientific Reports 8.1 (2018): 11943.

a/b twins as a $3\bar{2}$ stacking sequence inversion

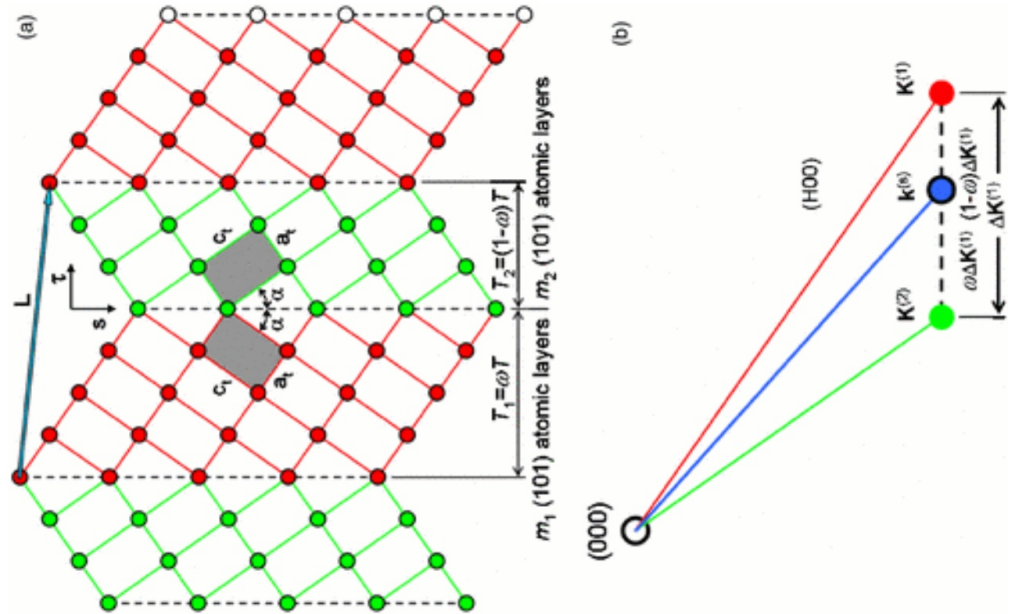
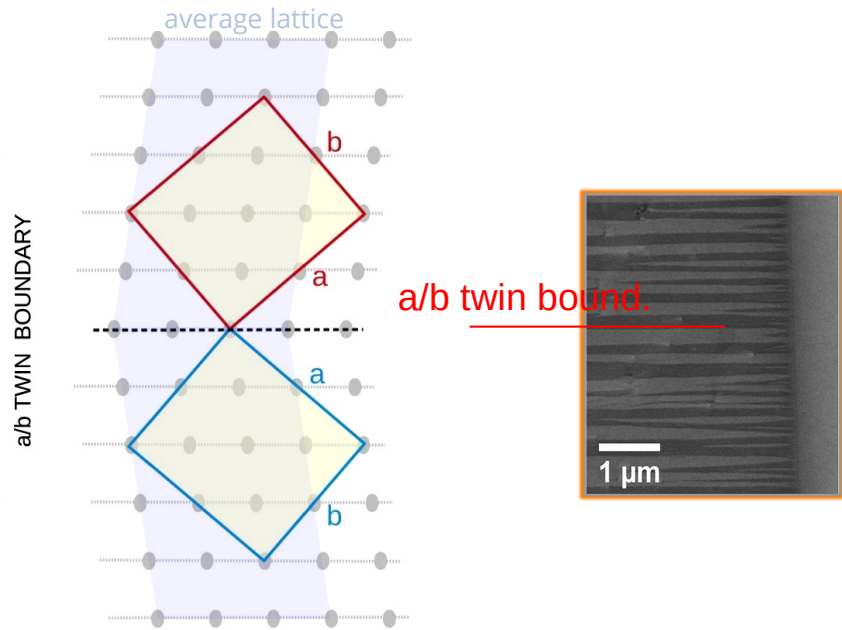
a/b twin boundary = stacking sequence inversion ... $3\bar{2}3\bar{2}3\bar{2}$ | $2\bar{3}2\bar{3}2\bar{3}$...



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a/b twins as a $3\bar{2}$ stacking sequence inversion

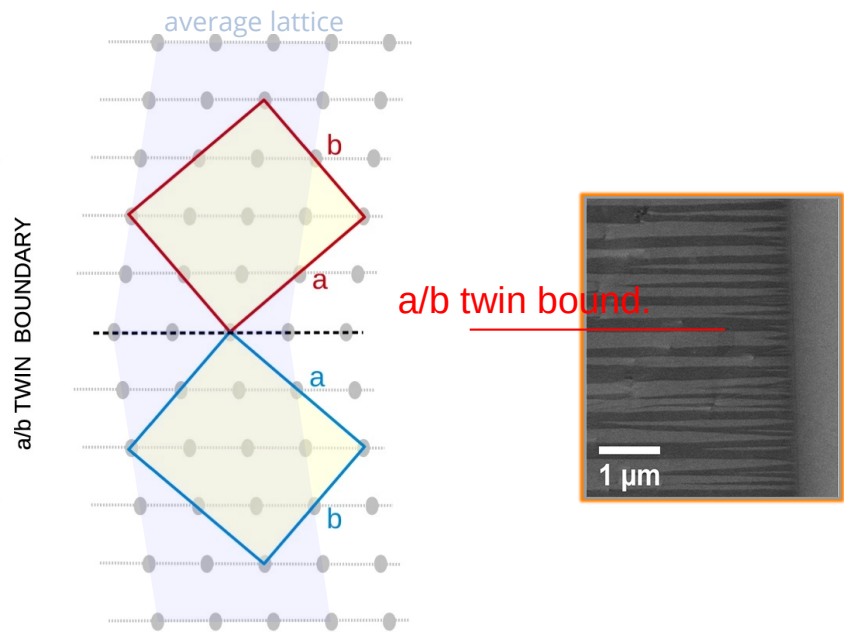
a/b twin boundary = stacking sequence inversion ... $3\bar{2}3\bar{2}3\bar{2}$ | $2\bar{3}2\bar{3}2\bar{3}$...



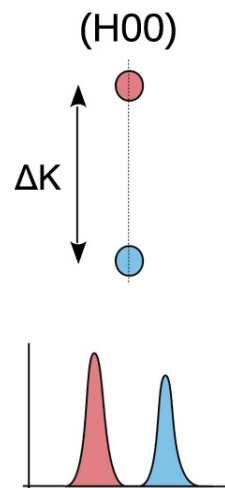
Yu U. Wang, Phys. Rev. B 74 (2006), 104109
 Yu U. Wang, Phys. Rev. B, 76 (2007), Article 024108

a/b twins as a $3\bar{2}$ stacking sequence inversion

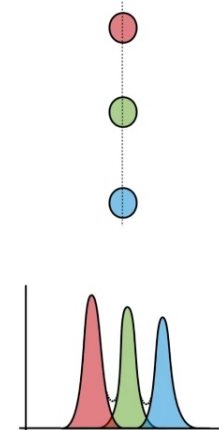
a/b twin boundary = stacking sequence inversion ... $3\bar{2}3\bar{2}3\bar{2}$ | $2\bar{3}2\bar{3}2\bar{3}$...



Coarse twins.



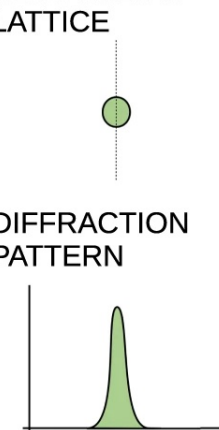
Intermediate size or mixture



Nanotwins

RECIPROCAL LATTICE

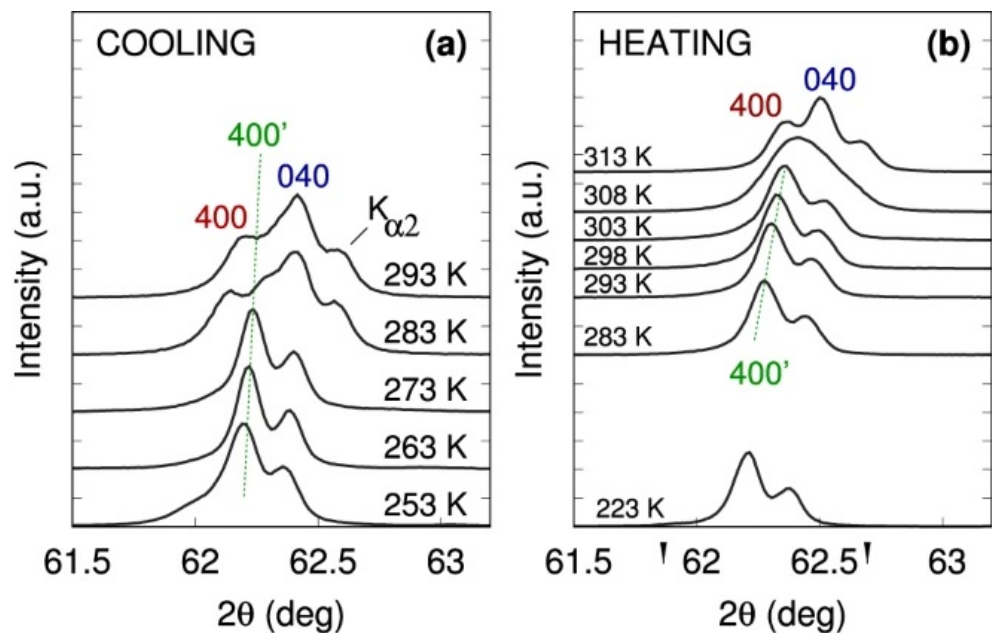
DIFFRACTION PATTERN



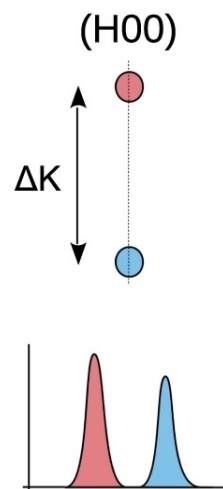
Straka, L., et al., Acta Materialia 132 (2017): 335-344.
Straka, L., et al., Scientific Reports 8.1 (2018): 11943.

a/b nanotwins as a $3\bar{2}$ stacking sequence inversion

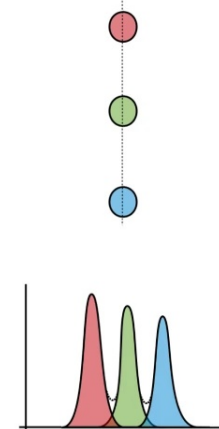
a/b twin boundary = stacking sequence inversion ... $3\bar{2}3\bar{2}3\bar{2}$ | $2\bar{3}2\bar{3}2\bar{3}$...



Coarse twins.



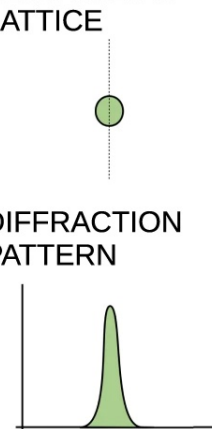
Intermediate size or mixture



Nanotwins

RECIPROCAL LATTICE

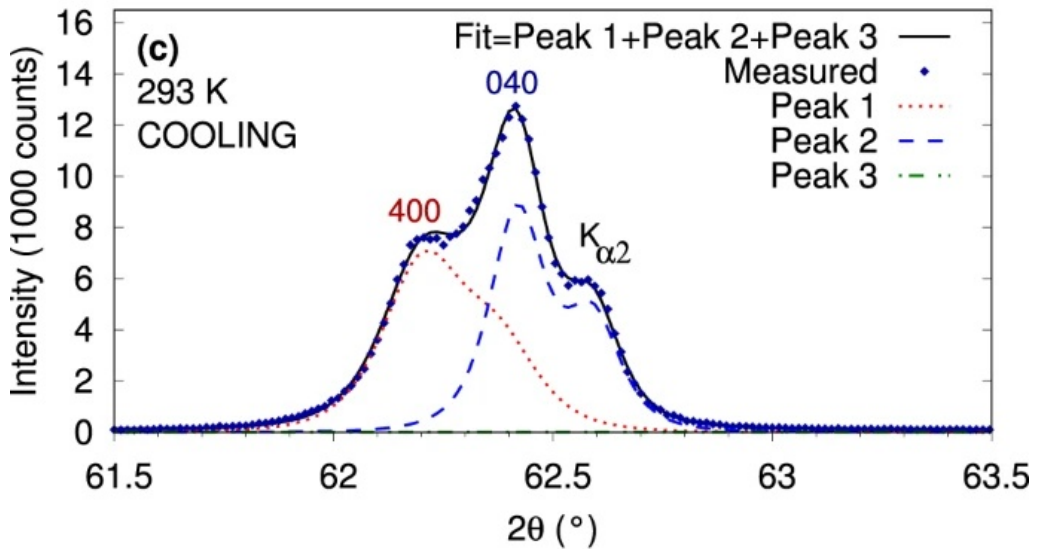
DIFFRACTION PATTERN



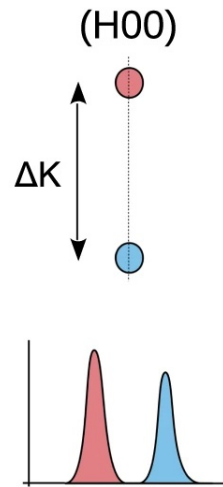
Straka, L., et al., Acta Materialia 132 (2017): 335-344.
Straka, L., et al., Scientific Reports 8.1 (2018): 11943.

a/b nanotwins as a $3\bar{2}$ stacking sequence inversion

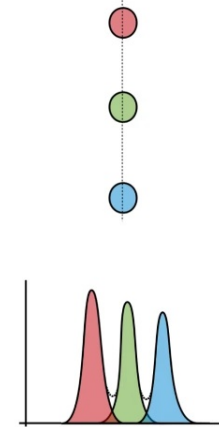
a/b twin boundary = stacking sequence inversion ... $3\bar{2}3\bar{2}3\bar{2}$ | $2\bar{3}2\bar{3}2\bar{3}$...



Coarse twins.



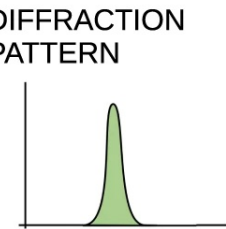
Intermediate size or mixture



Nanotwins

RECIPROCAL LATTICE

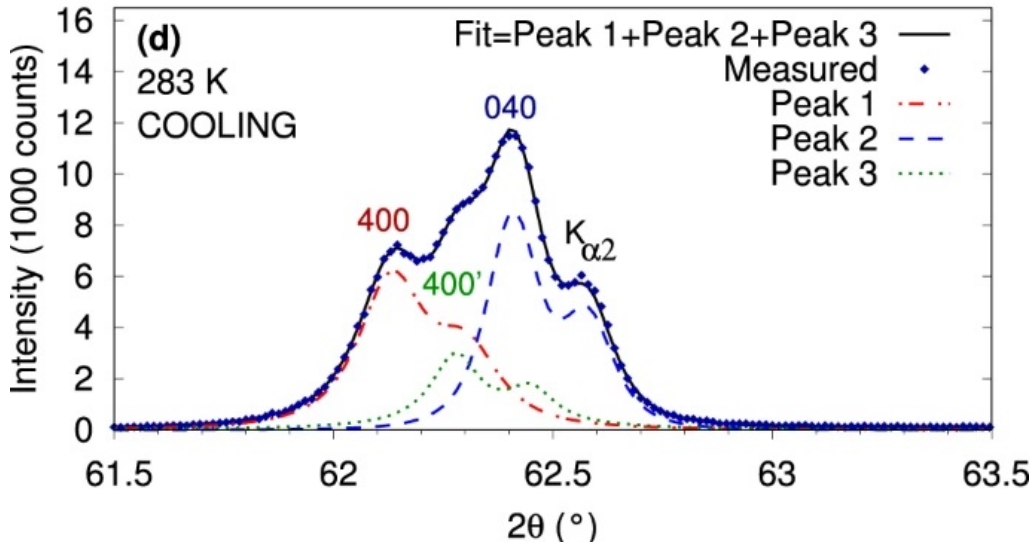
DIFFRACTION PATTERN



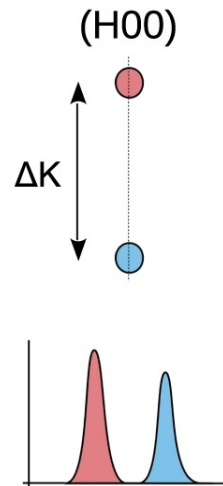
Straka, L., et al., Acta Materialia 132 (2017): 335-344.
 Straka, L., et al., Scientific Reports 8.1 (2018): 11943.

a/b nanotwins as a $3\bar{2}$ stacking sequence inversion

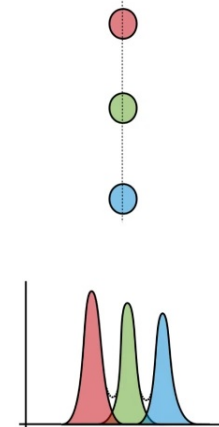
a/b twin boundary = stacking sequence inversion ... $3\bar{2}3\bar{2}3\bar{2}$ | $2\bar{3}2\bar{3}2\bar{3}$...



Coarse twins.



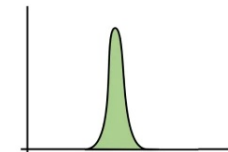
Intermediate size or mixture



Nanotwins

RECIPROCAL LATTICE

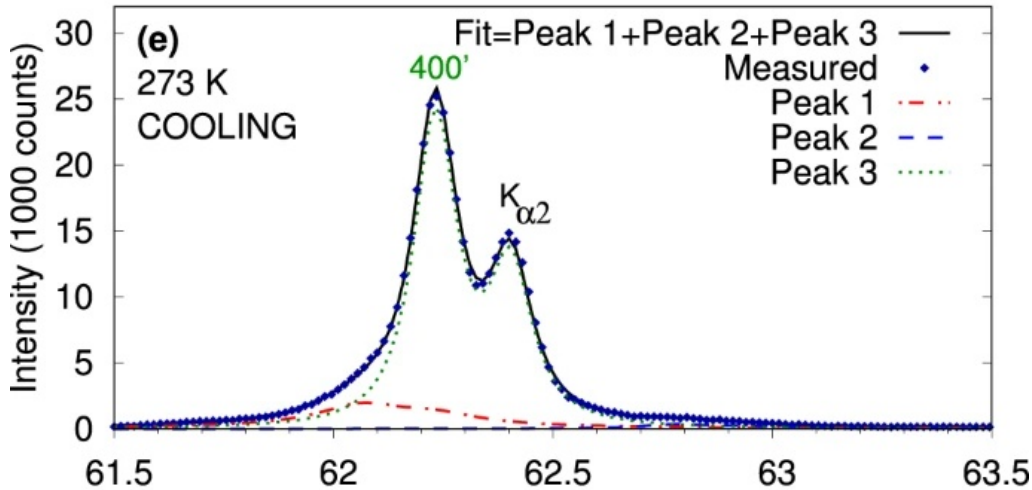
DIFFRACTION PATTERN



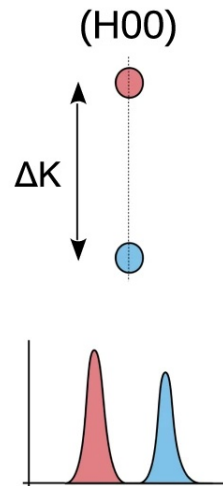
Straka, L., et al., Acta Materialia 132 (2017): 335-344.
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a/b nanotwins as a $3\bar{2}$ stacking sequence inversion

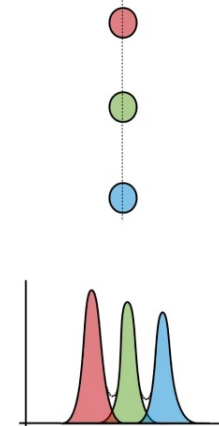
a/b twin boundary = stacking sequence inversion ... $3\bar{2}3\bar{2}3\bar{2}$ | $2\bar{3}2\bar{3}2\bar{3}$...



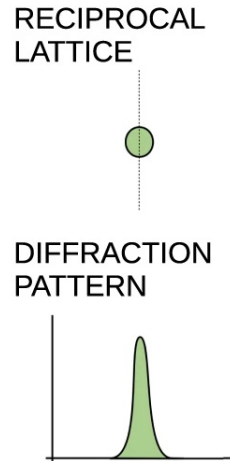
Coarse twins.



Intermediate size or mixture



Nanotwins



a/b nanotwins as a $3\bar{2}$ stacking sequence inversion

a/b twin boundary = stacking sequence inversion ... $3\bar{2}3\bar{2}3\bar{2}$ | $2\bar{3}2\bar{3}2\bar{3}$...

Nanotwins - adaptive diffraction condition:

$$m < 2/sH$$

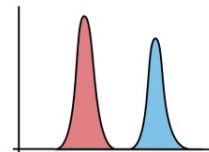
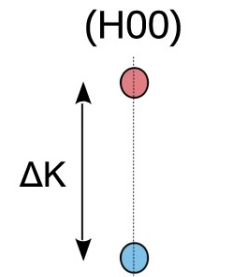
where $s = 0.0045$ is twinning shear and $H = 4$ is reciprocal space coordinate

=>

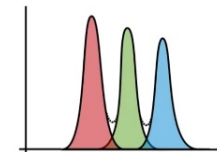
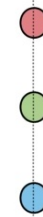
size of a/b twin

$$m < 20 \text{ nm (100 atomic planes)}$$

Coarse twins.



Intermediate size or mixture

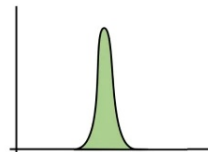


Nanotwins

RECIPROCAL LATTICE



DIFFRACTION PATTERN



a/b nanotwins as a $3\bar{2}$ stacking sequence inversion

Nanotwins - adaptive diffraction condition:

$$m < 2/sH$$

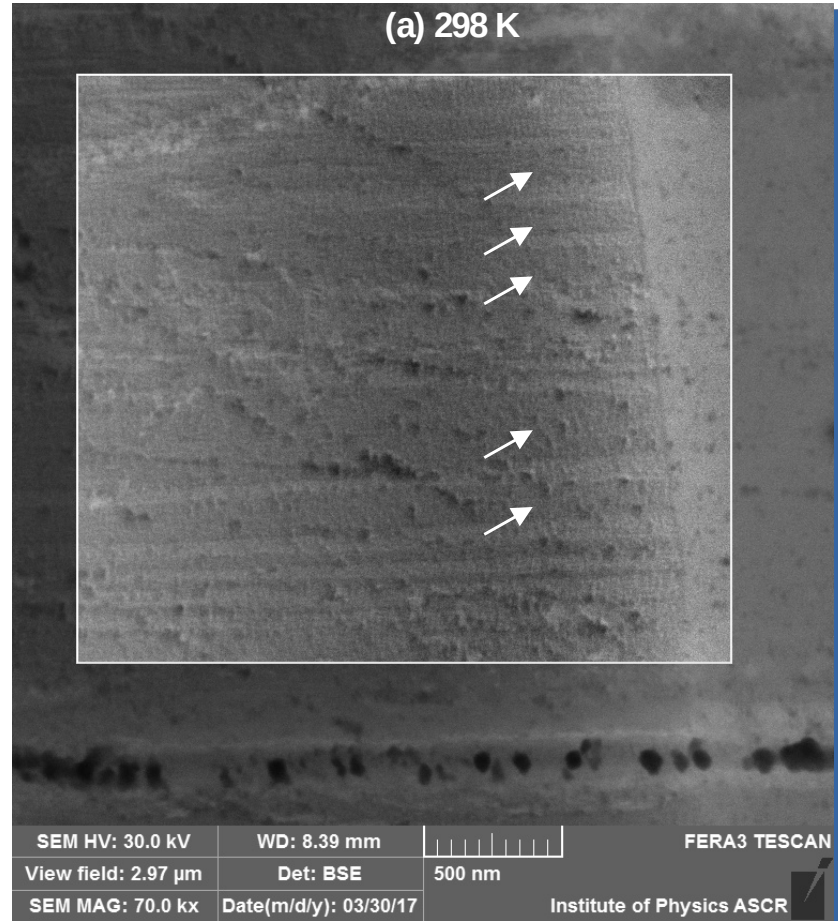
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a/b nanotwins as a $3\bar{2}$ stacking sequence inversion

Nanotwins - adaptive diffraction condition:

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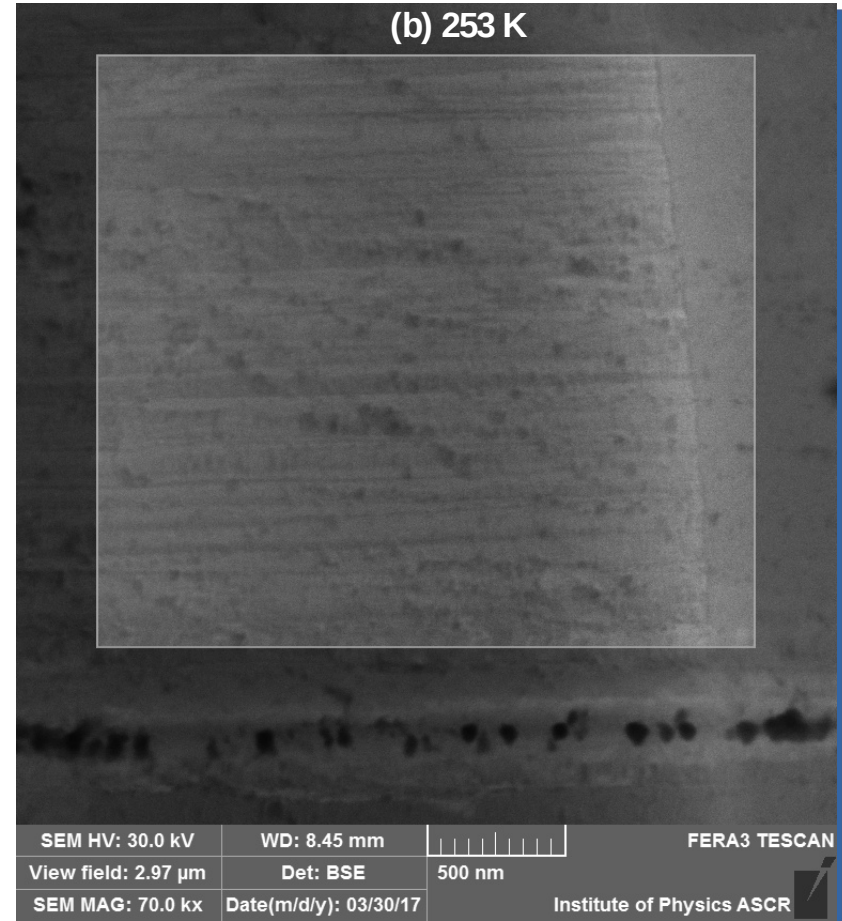
where $s = 0.0045$ is twinning shear and $H = 4$ is reciprocal space coordinate

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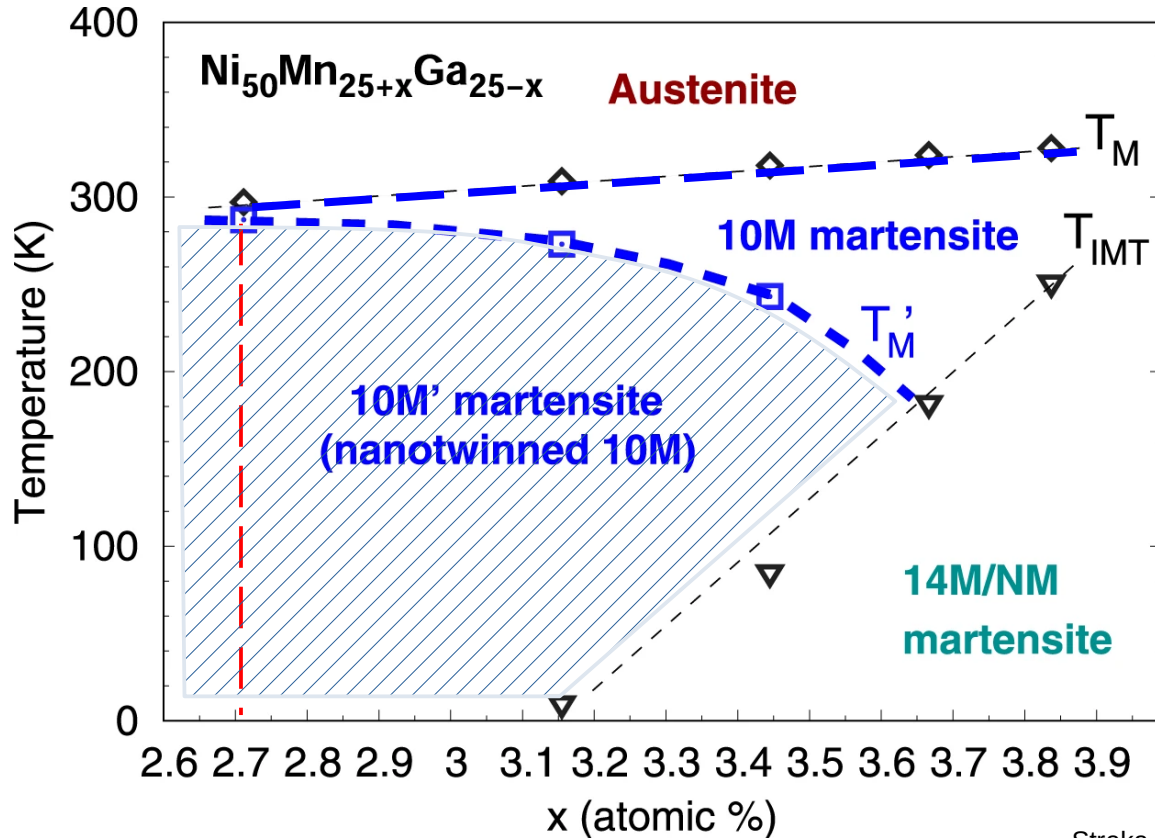
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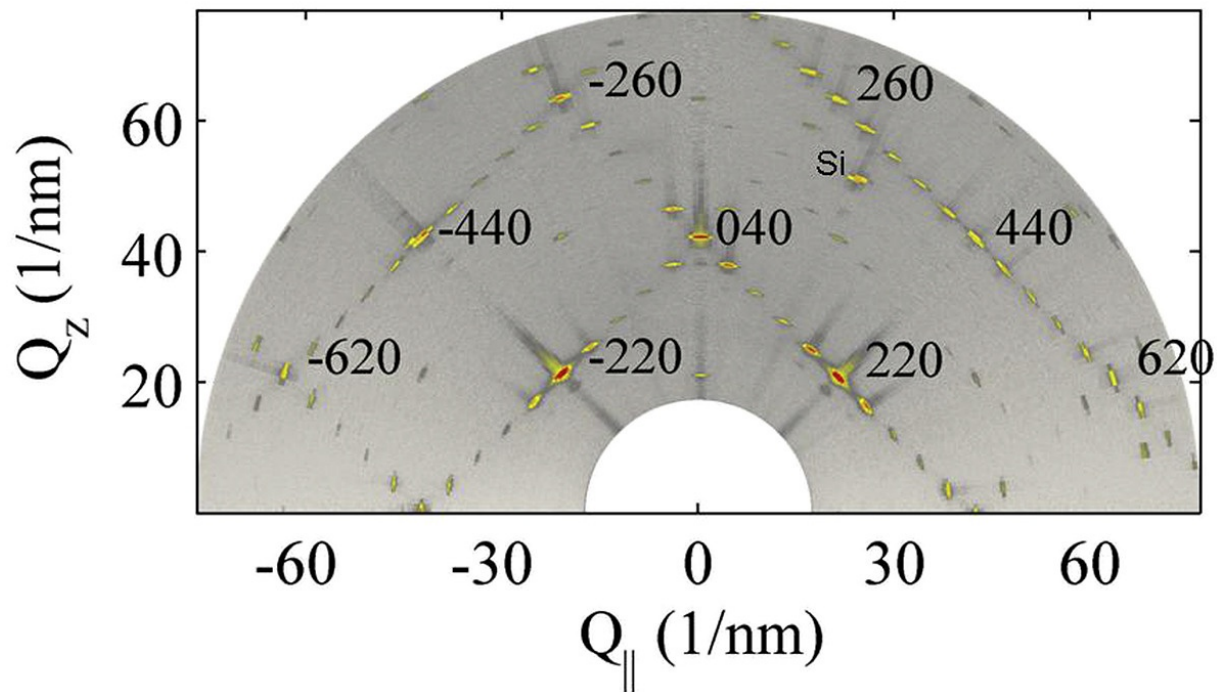
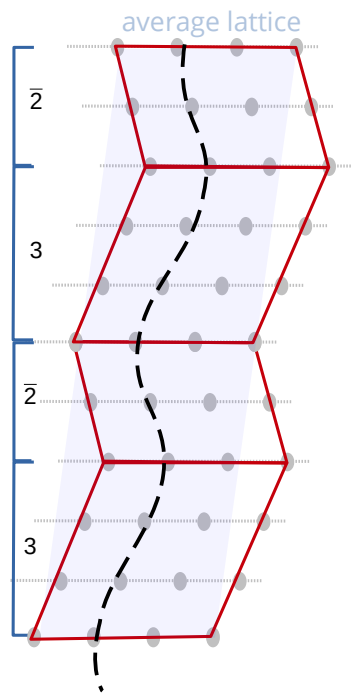


a/b nanotwins as a $3\bar{2}$ stacking sequence inversion



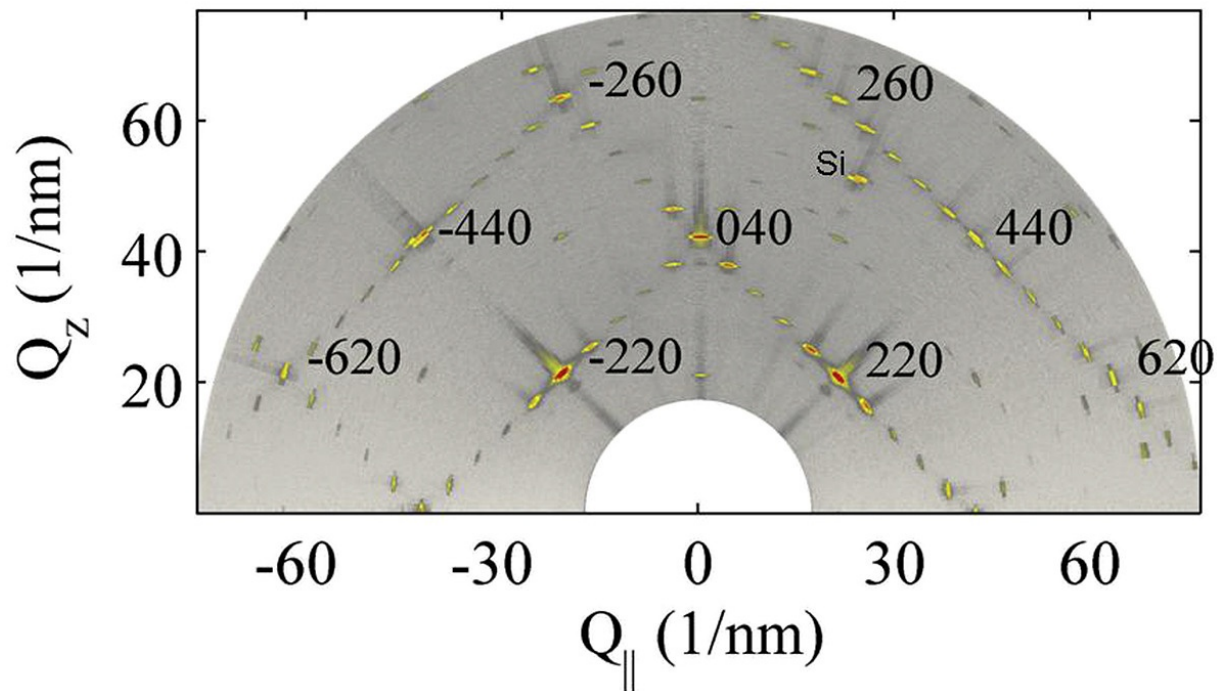
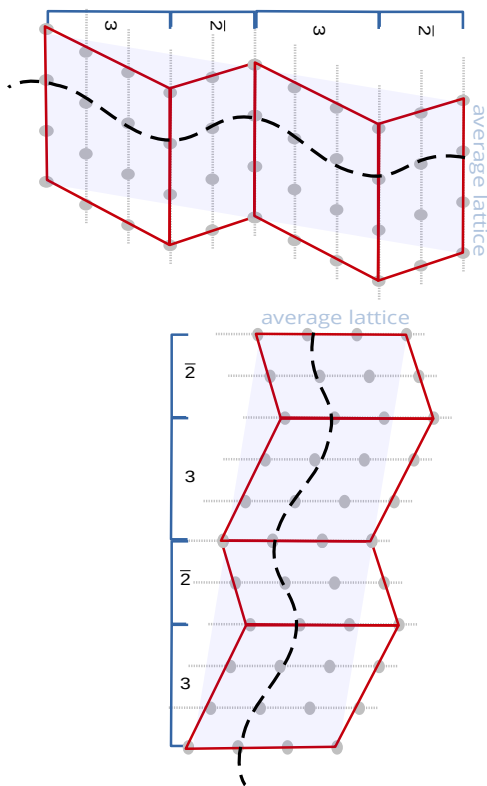
Straka, L., et al., Acta Materialia 132 (2017): 335-344.
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Modulation



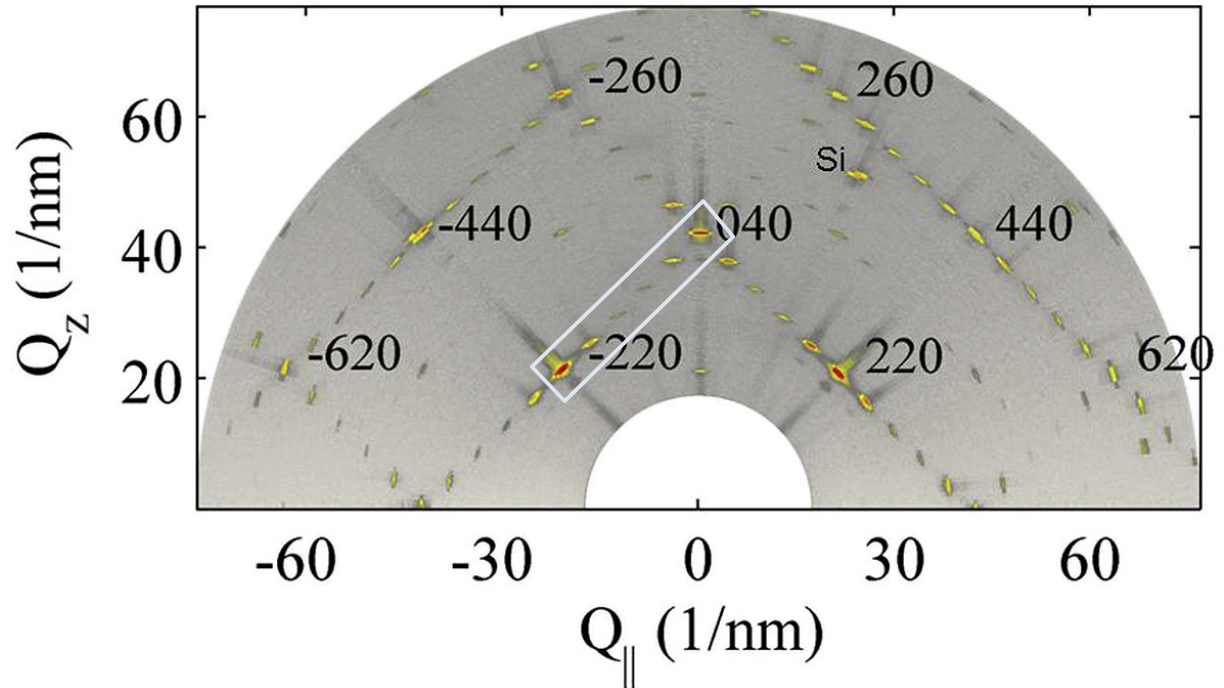
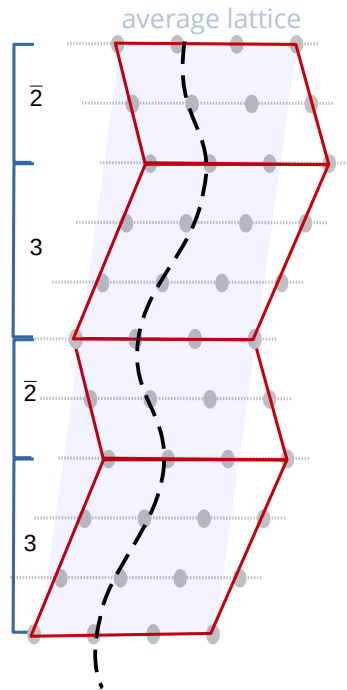
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Modulation



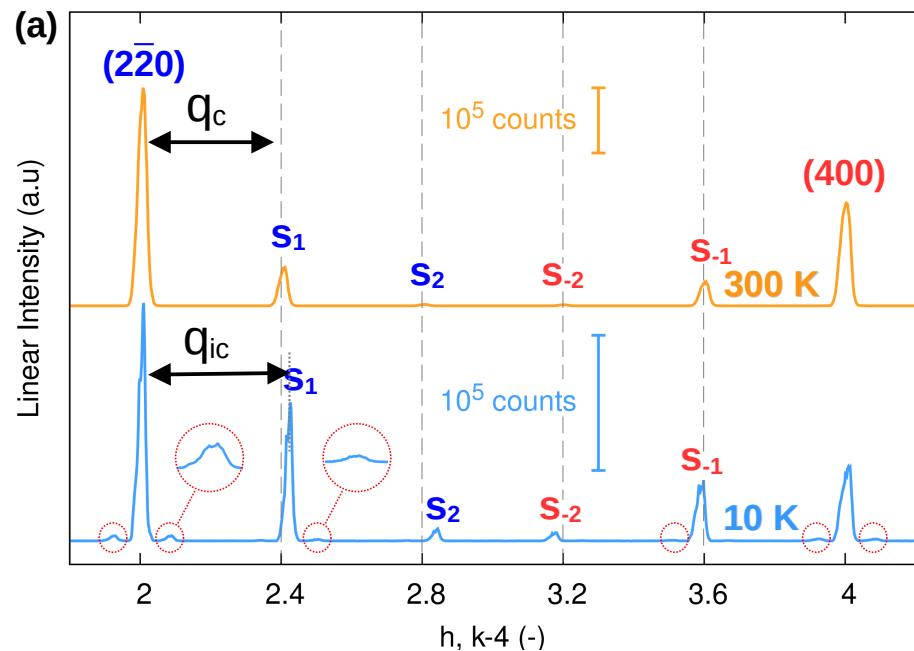
Heczko, Oleg, et al. Acta Materialia 115 (2016): 250-258.

Modulation – study by high-resolution q-scan



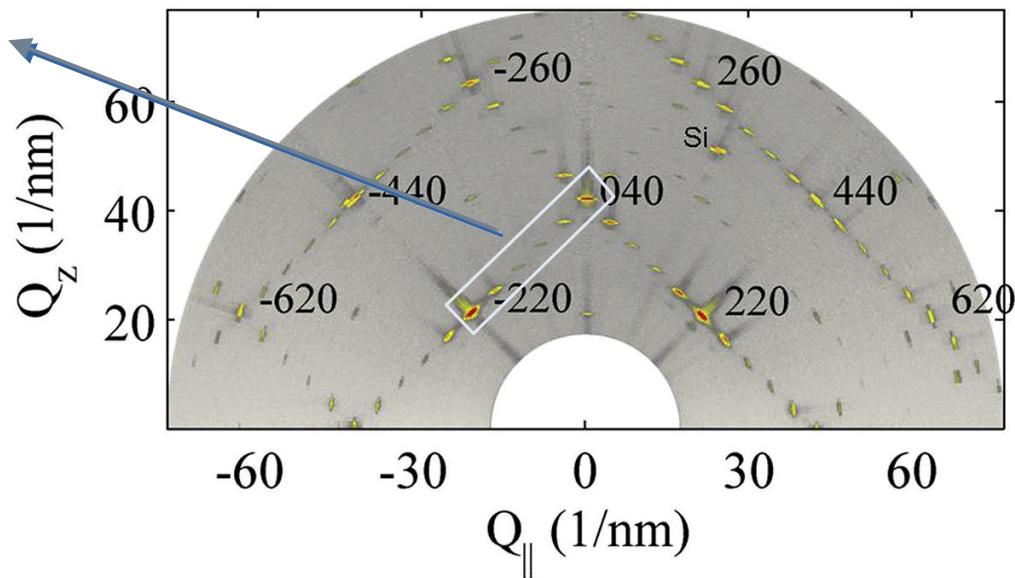
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Modulation – study by high-resolution q-scan

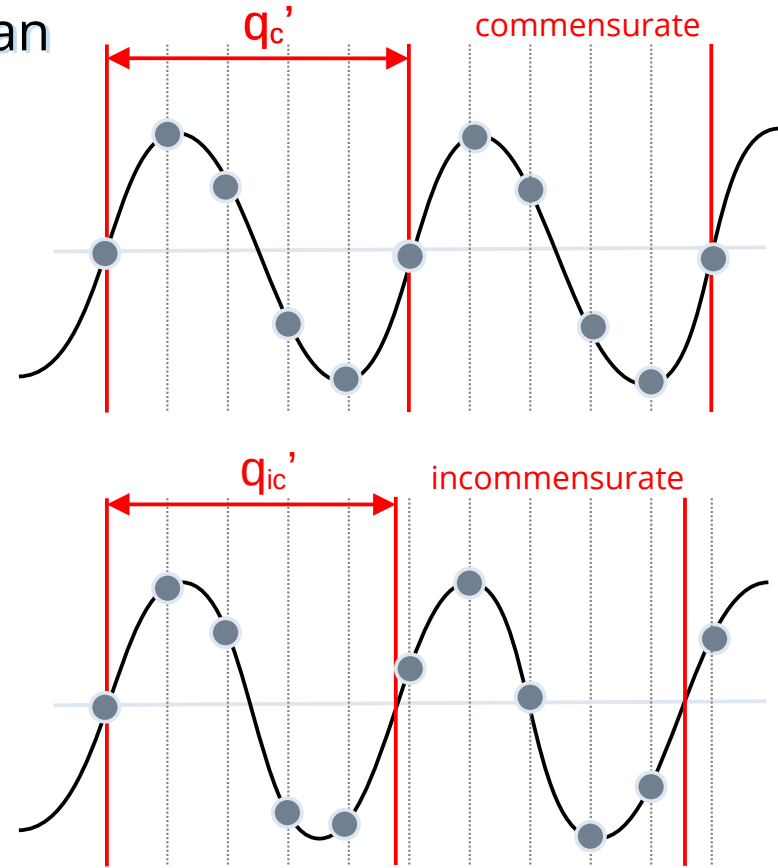
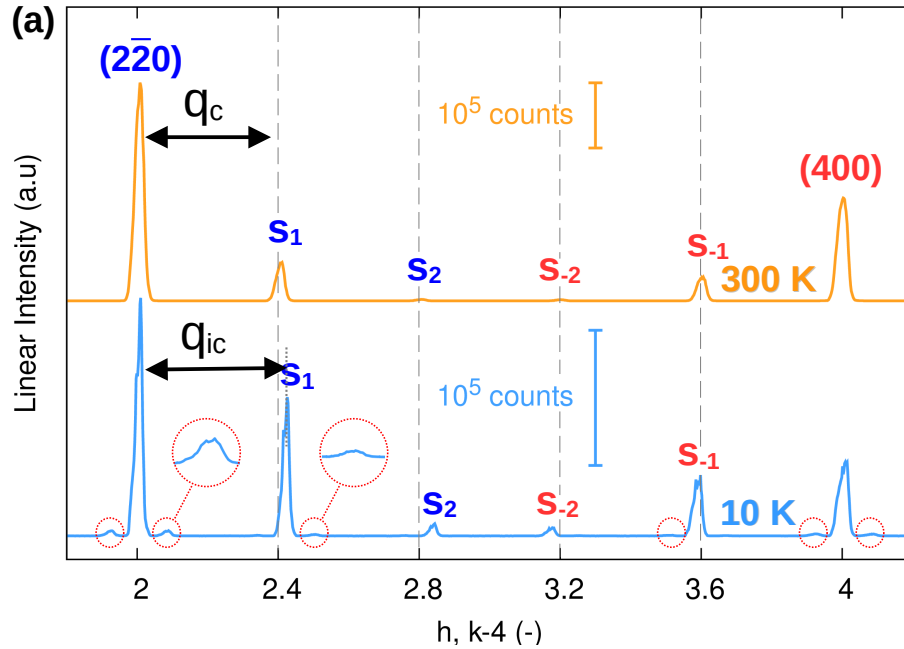


$$\mathbf{q} = (q, q, 0)$$

$$q' = 2/q$$



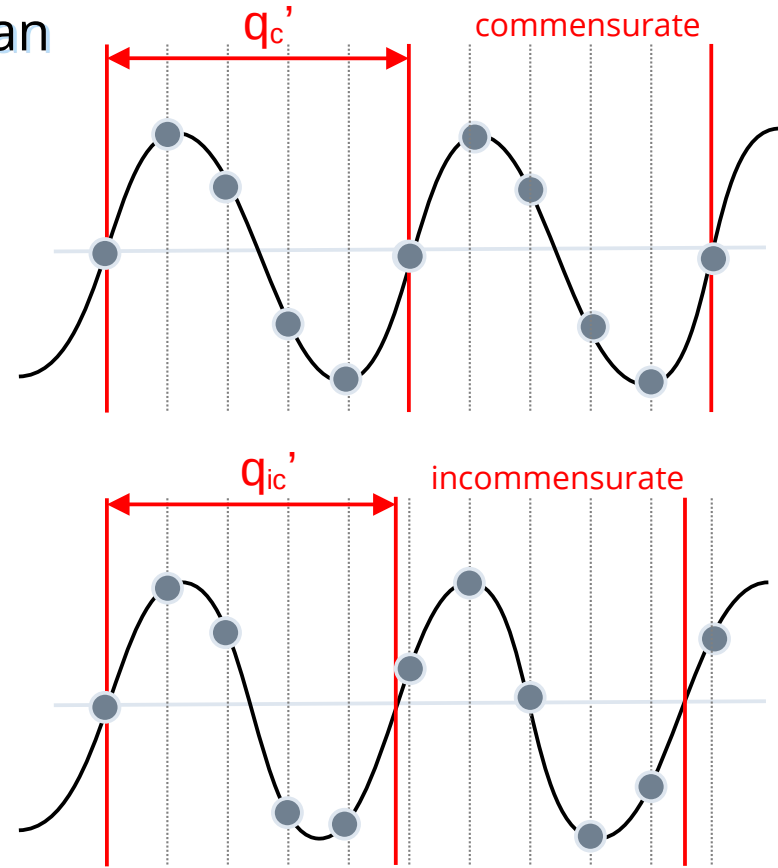
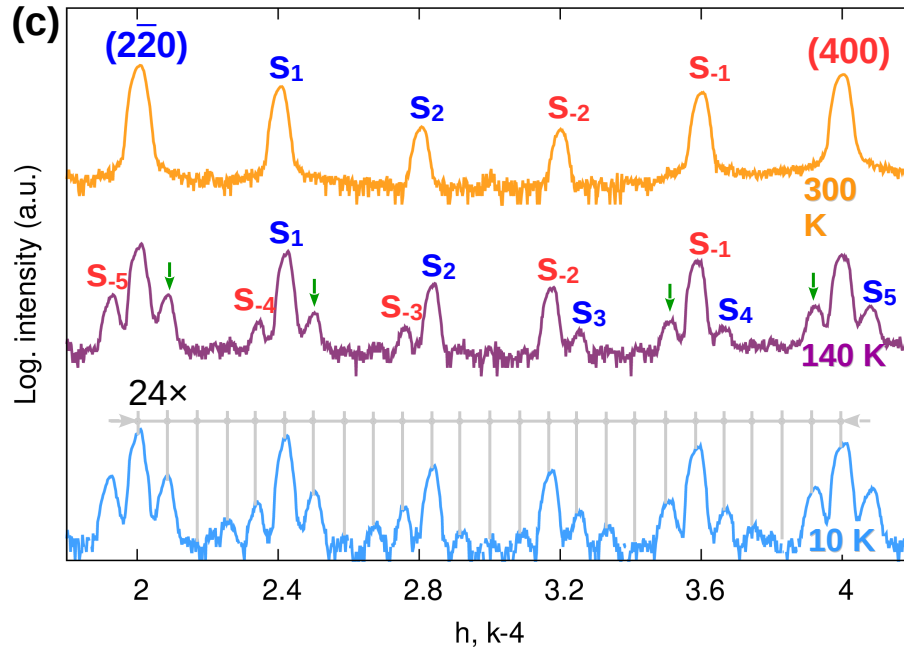
Modulation – study by high-resolution q-scan



$$\mathbf{q} = (q, q, 0)$$

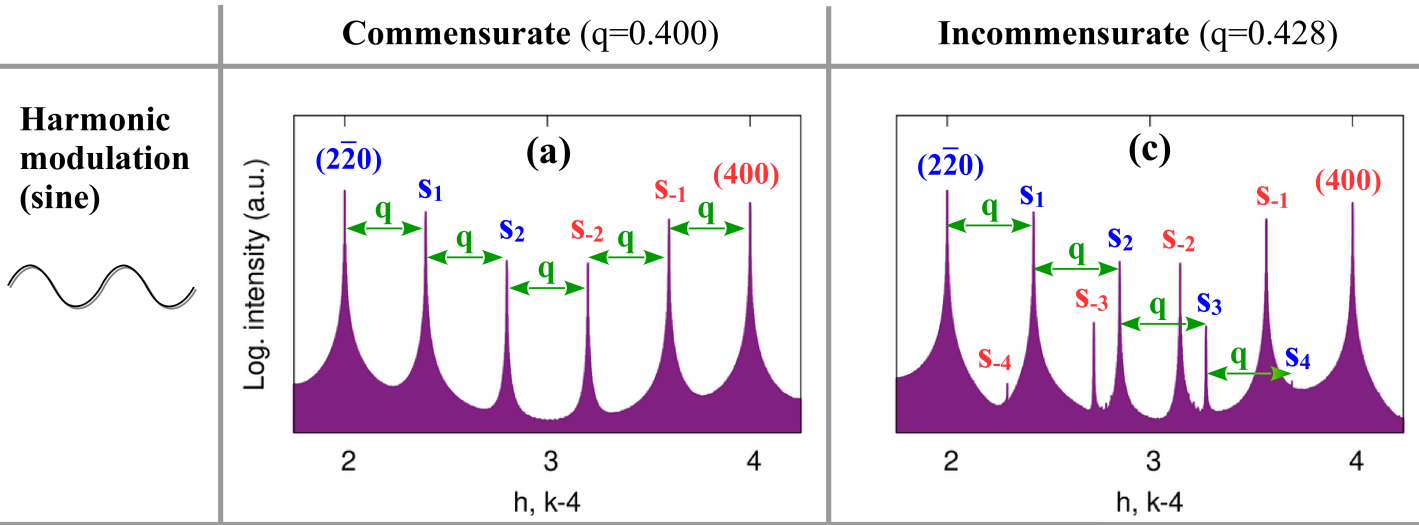
$$q' = 2/q$$

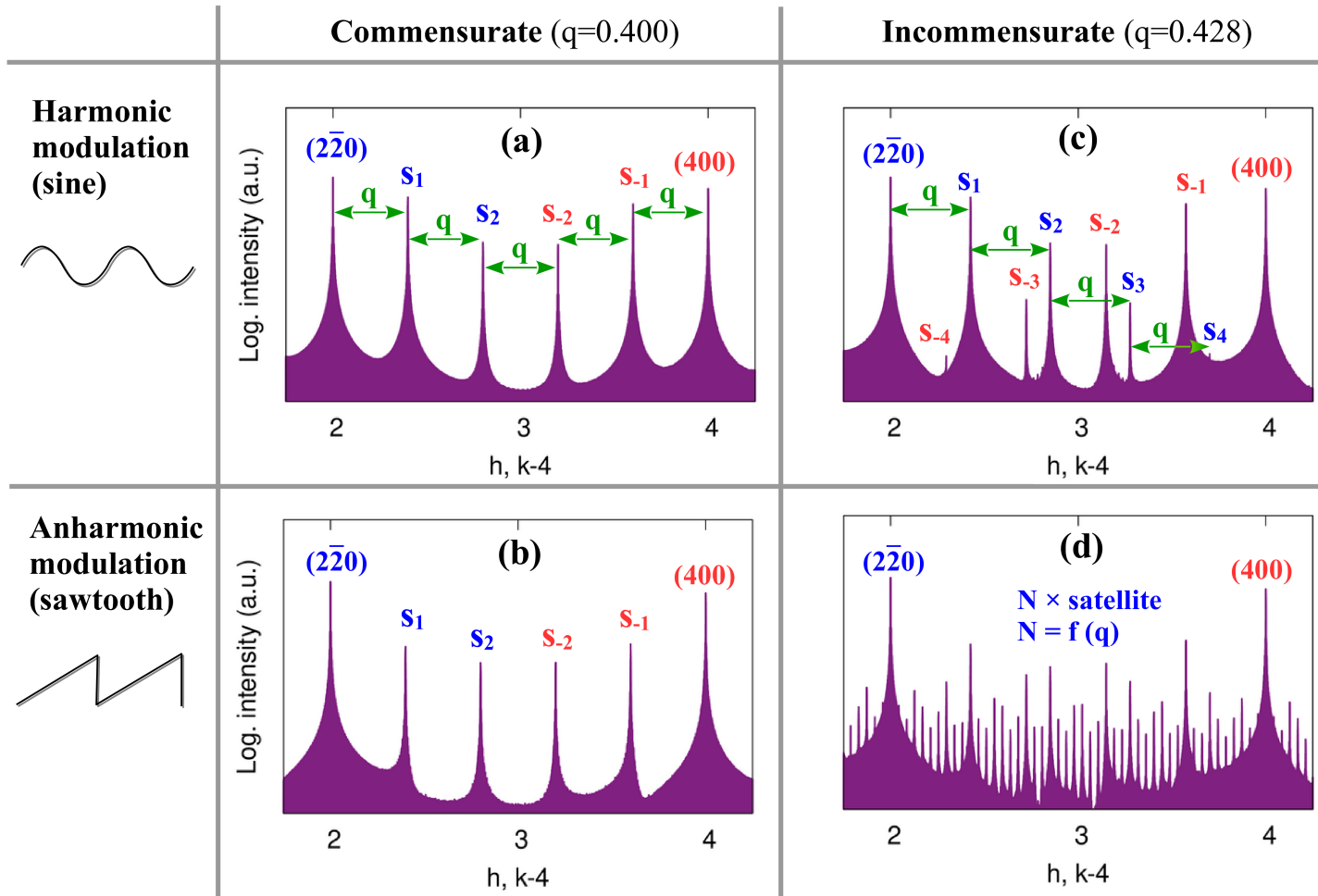
Modulation – study by high-resolution q-scan



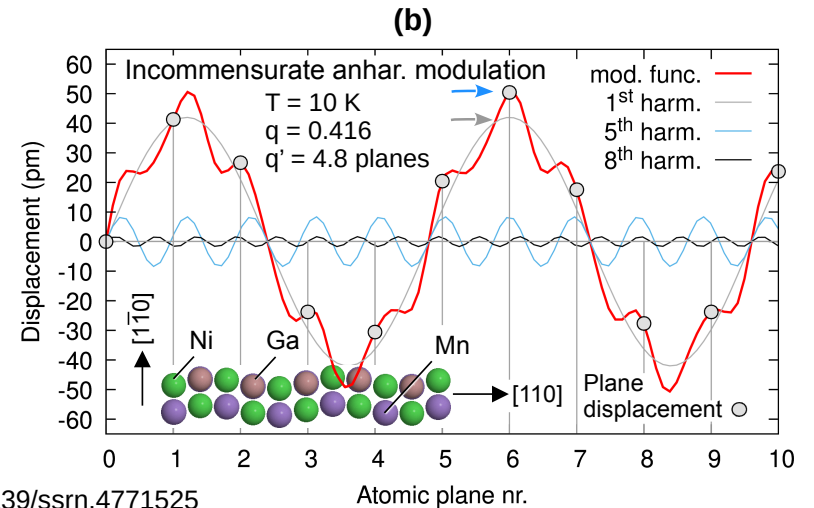
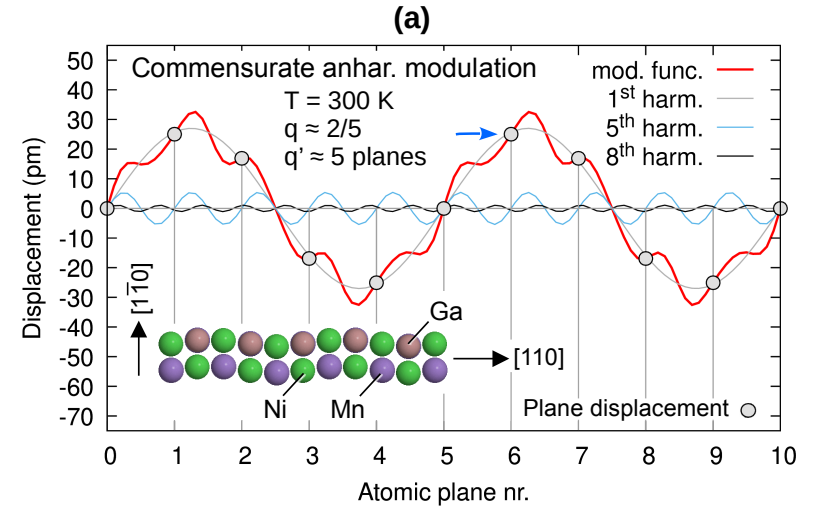
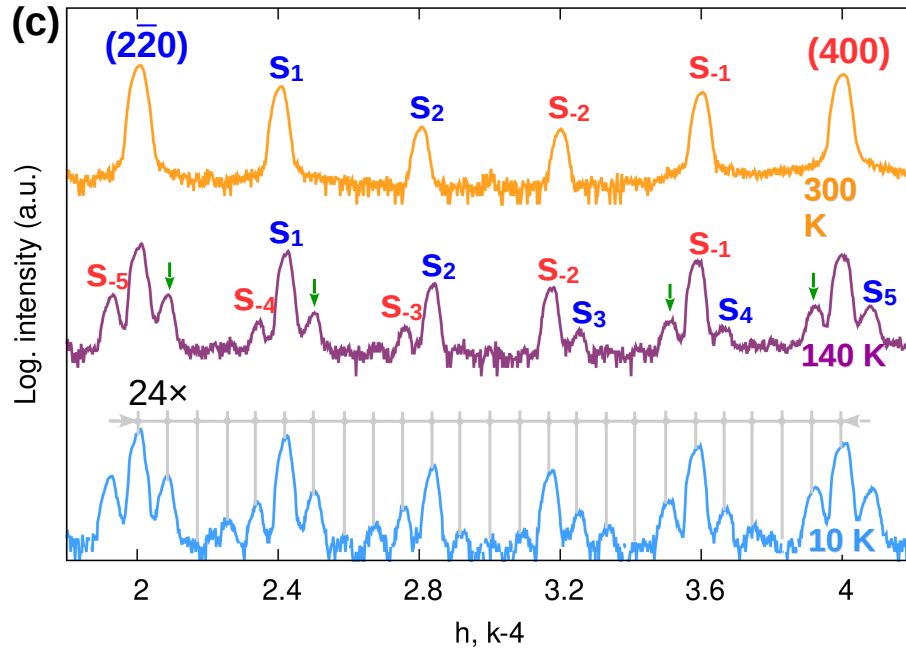
$$\mathbf{q}=(q,q,0)$$

$$q'=2/q$$

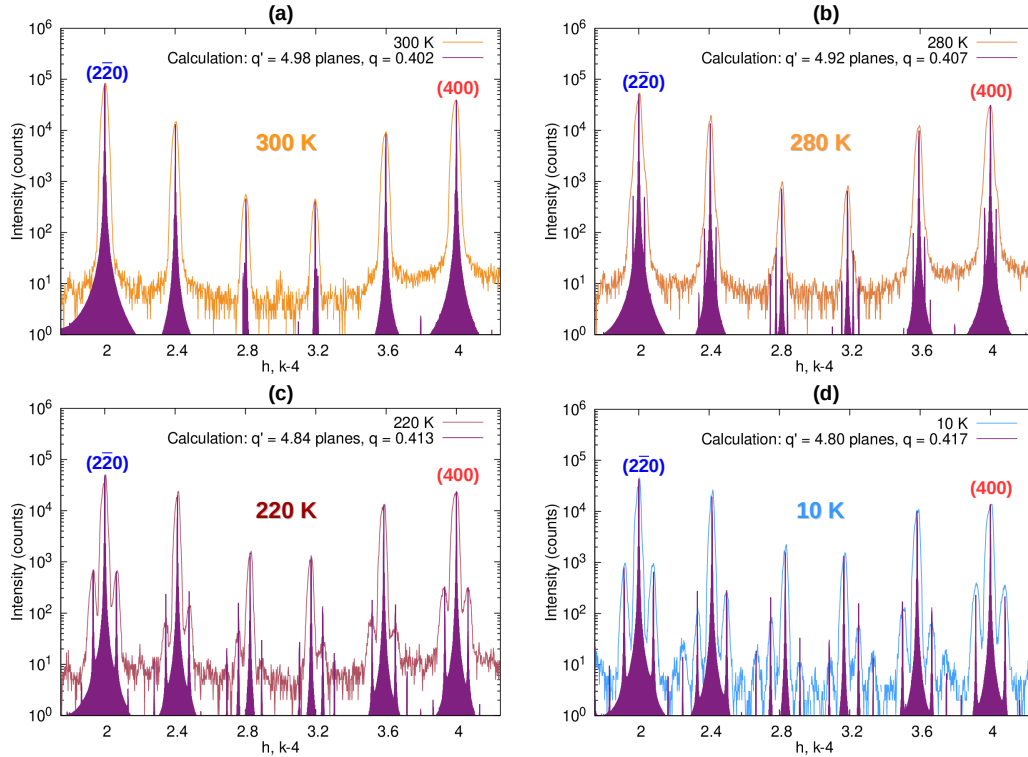




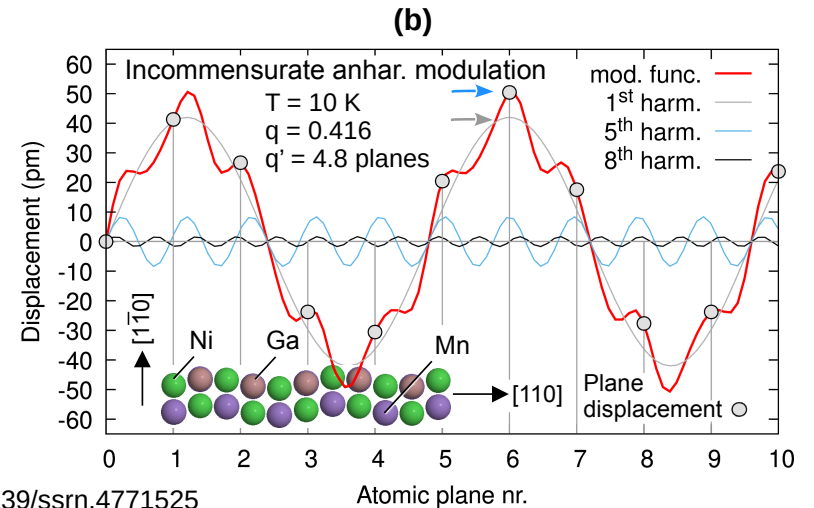
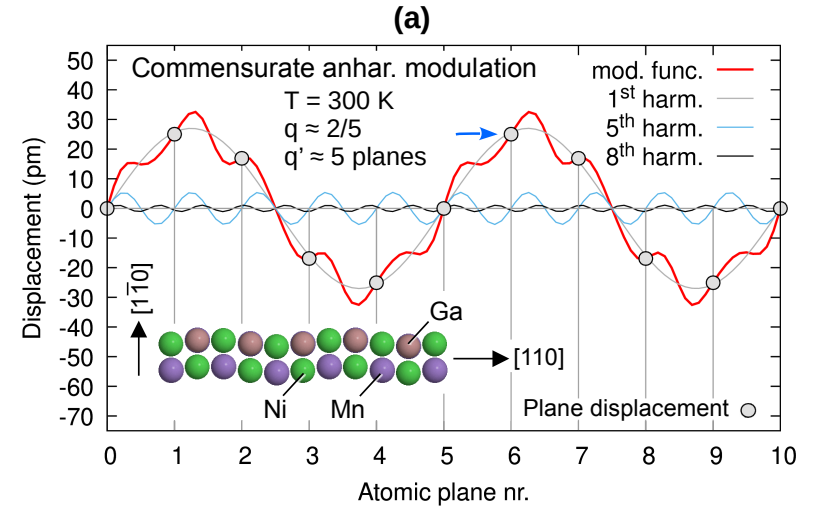
Modulation – study by high-resolution q-scan



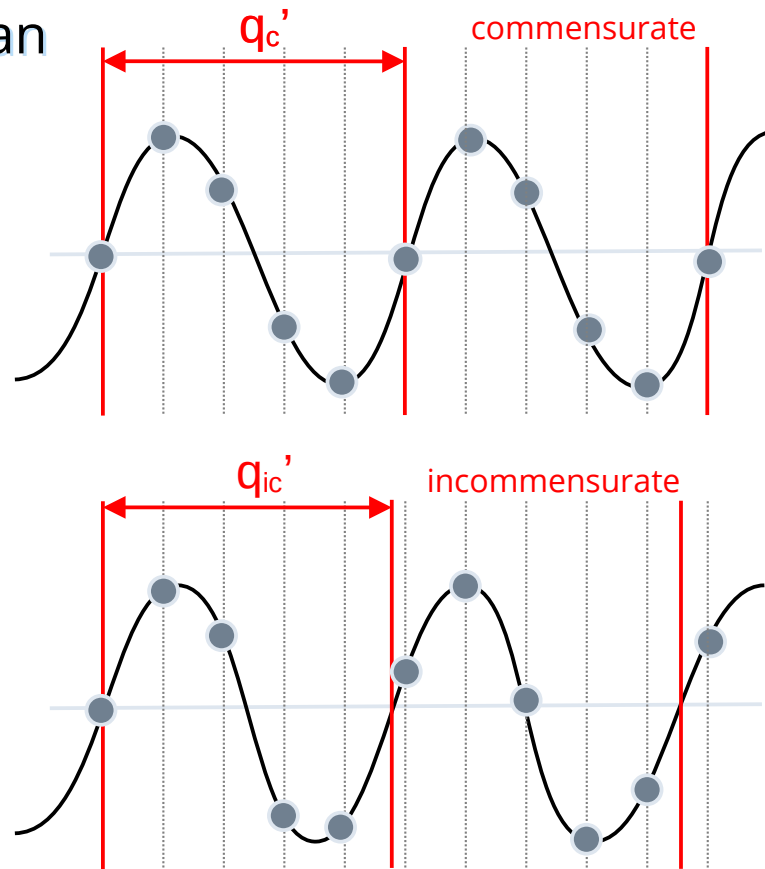
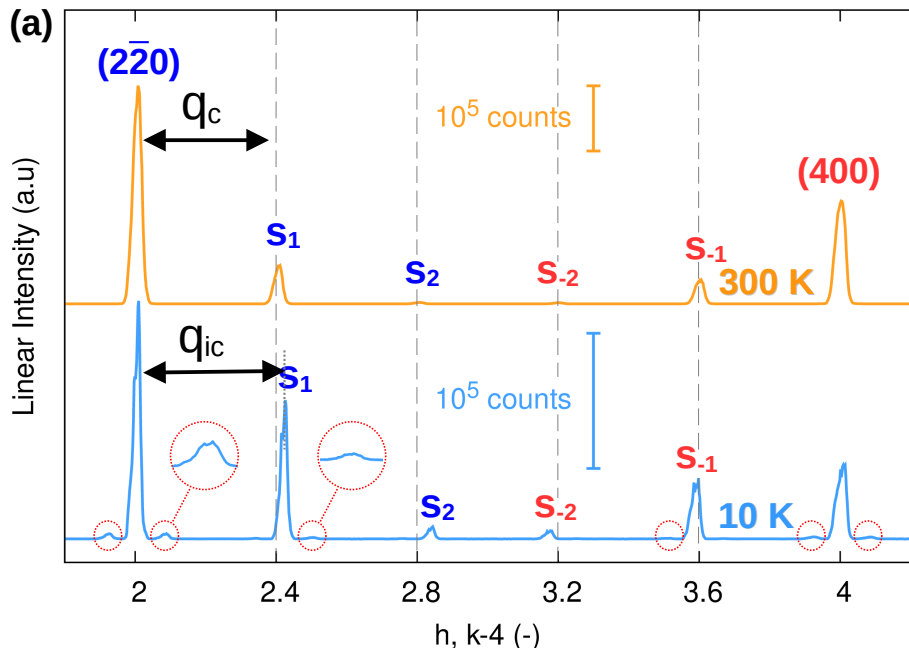
Modulation – study by high-resolution q-scan



$$HKL(T) = f(q(T))$$



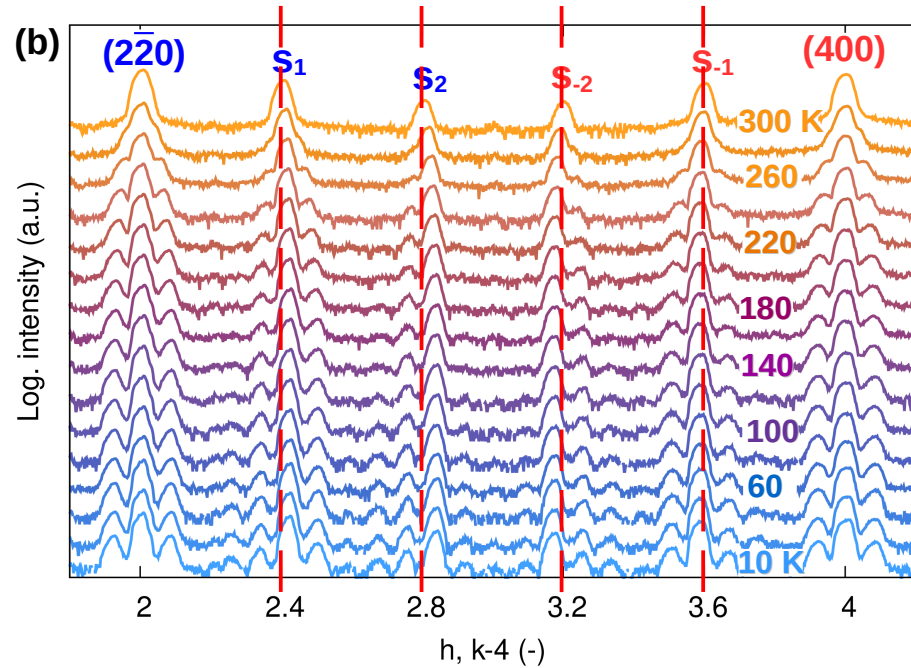
Aperiodicity – study by high-resolution q-scan



$$\mathbf{q} = (q, q, 0)$$

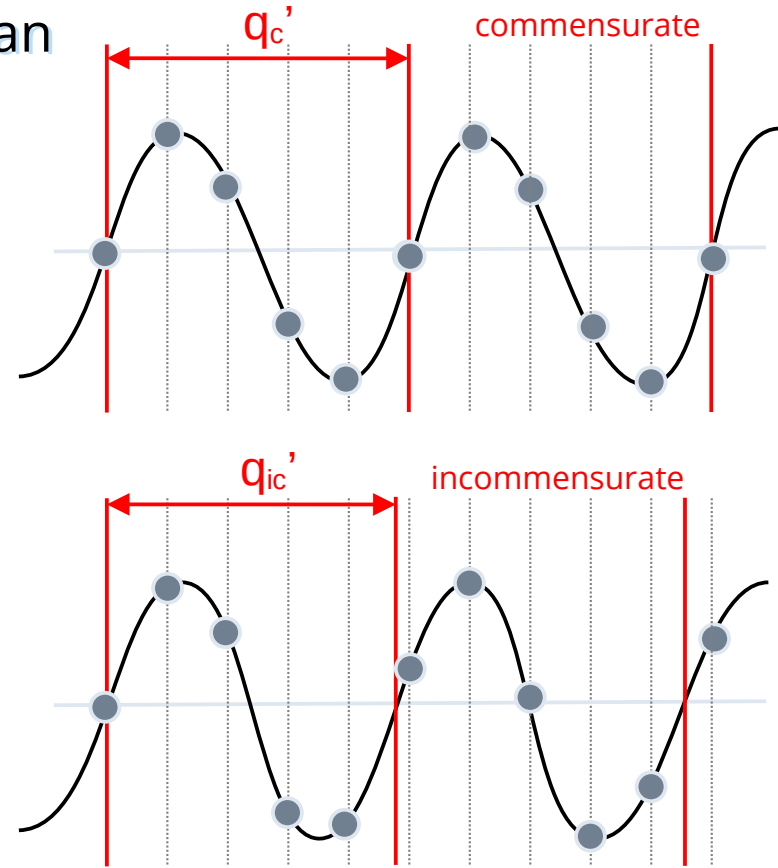
$$q' = 2/q$$

Aperiodicity – study by high-resolution q-scan

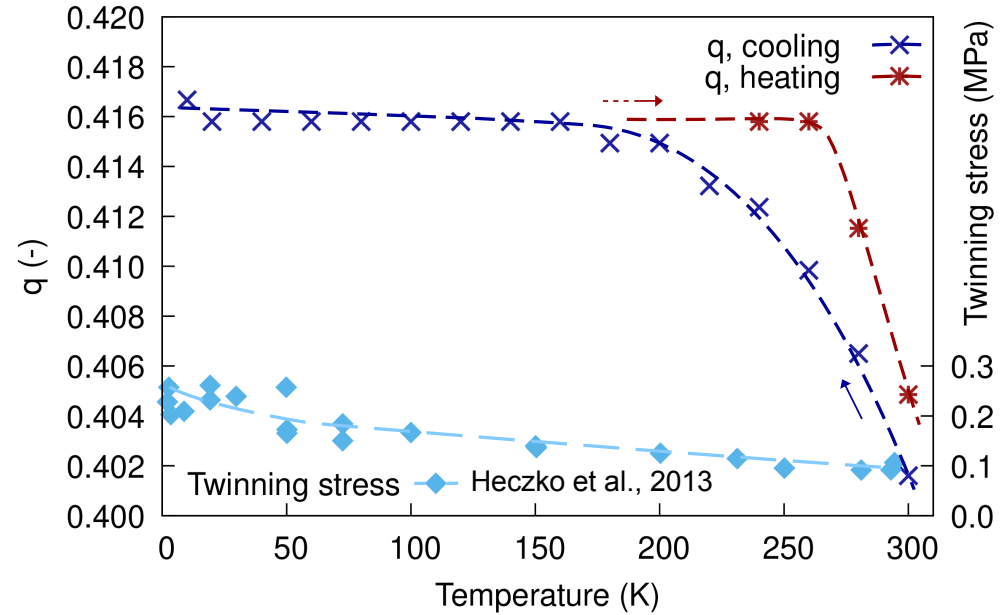
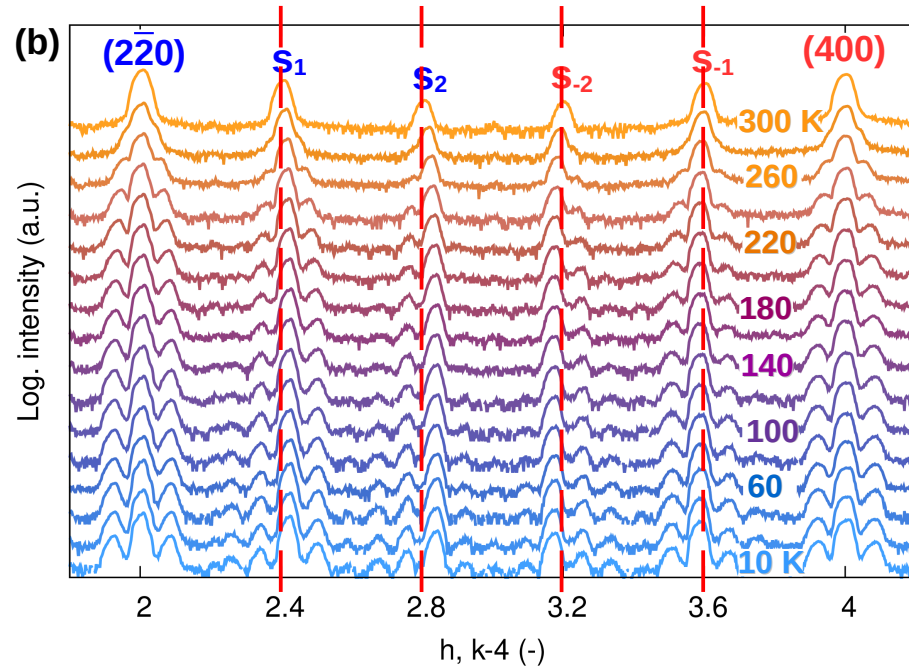


$$\mathbf{q} = (q, q, 0)$$

$$q' = 2/q$$



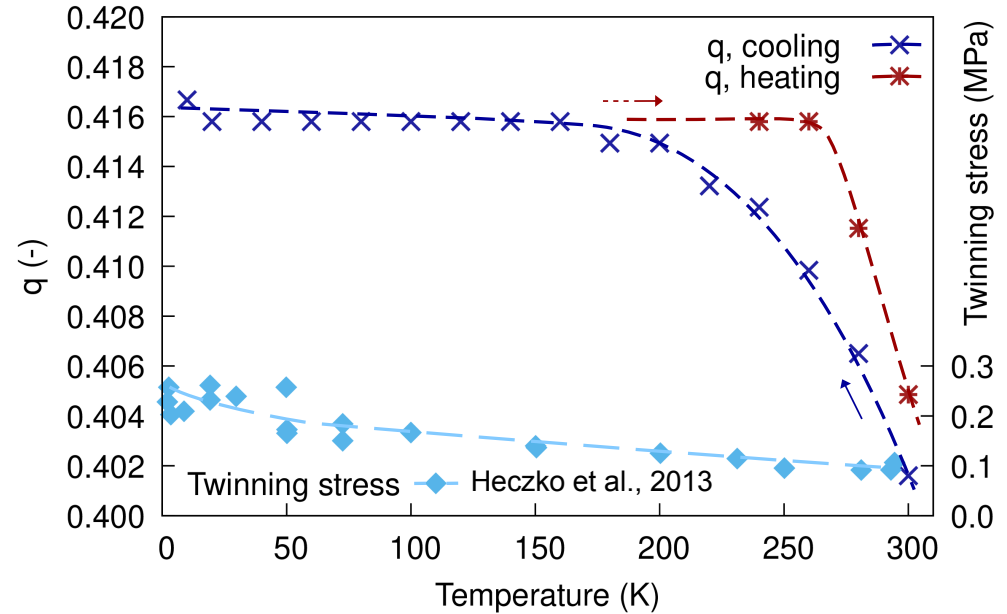
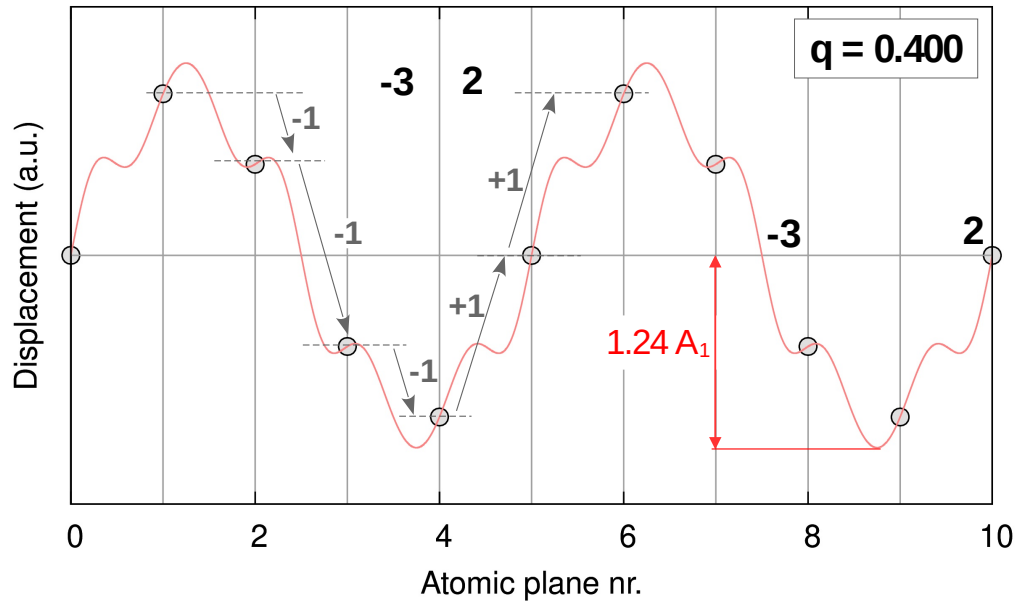
Aperiodicity – study by high-resolution q-scan



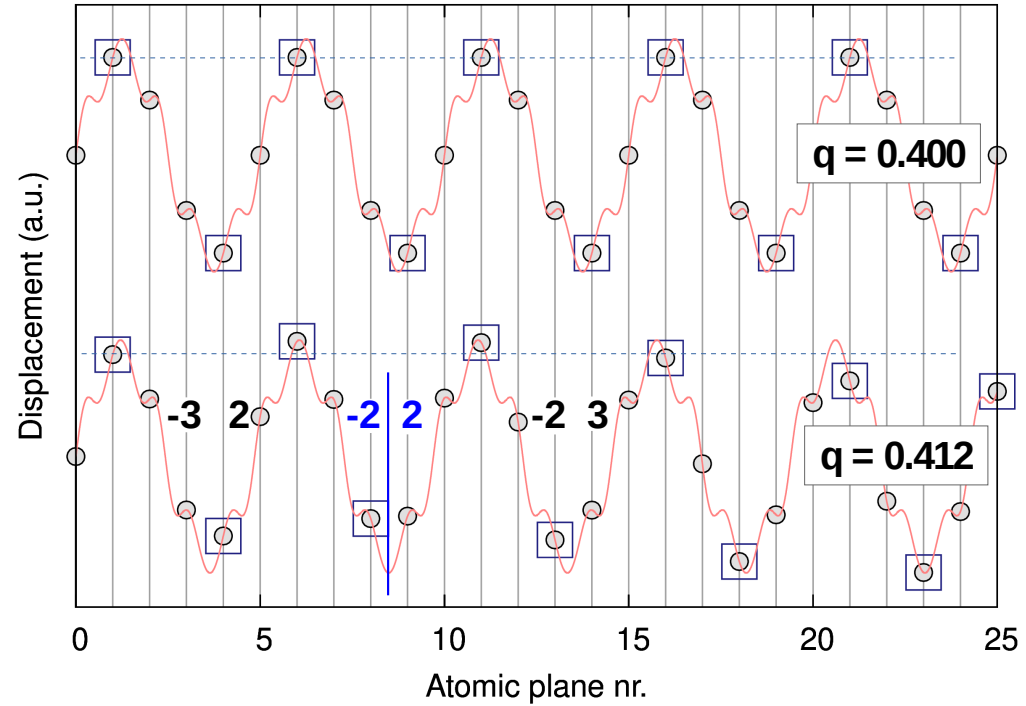
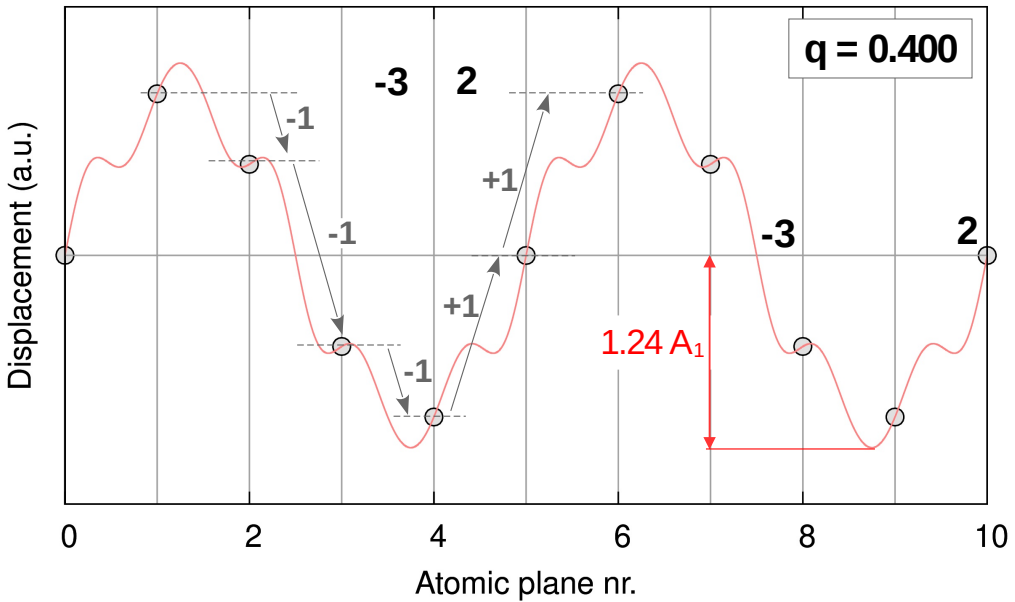
$$\mathbf{q}=(q,q,0)$$

$$q'=2/q$$

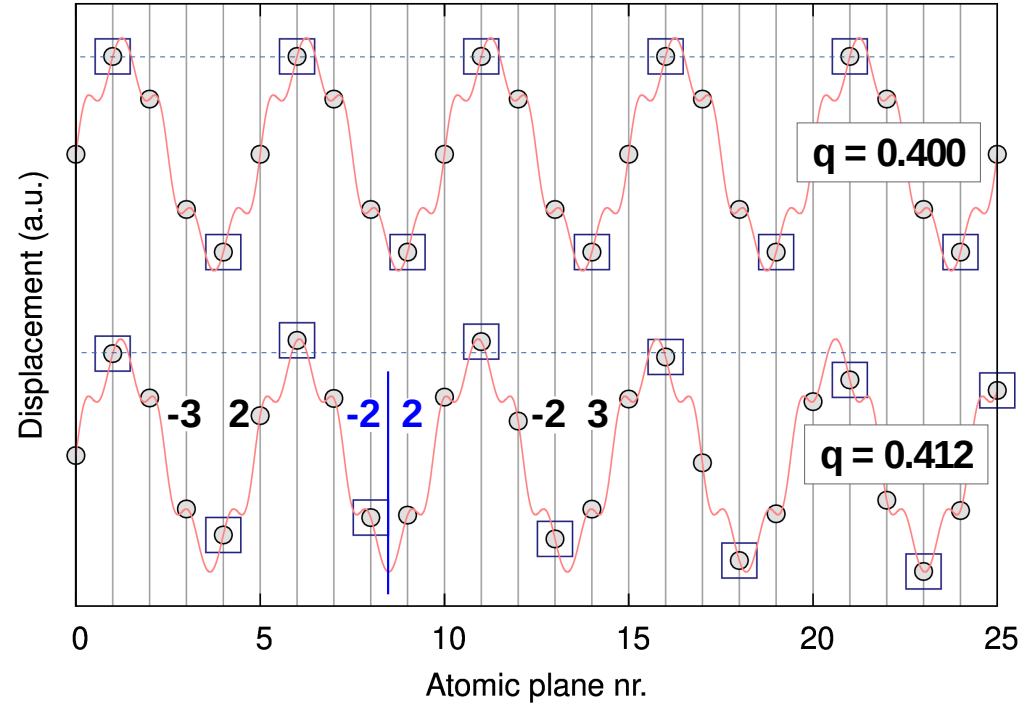
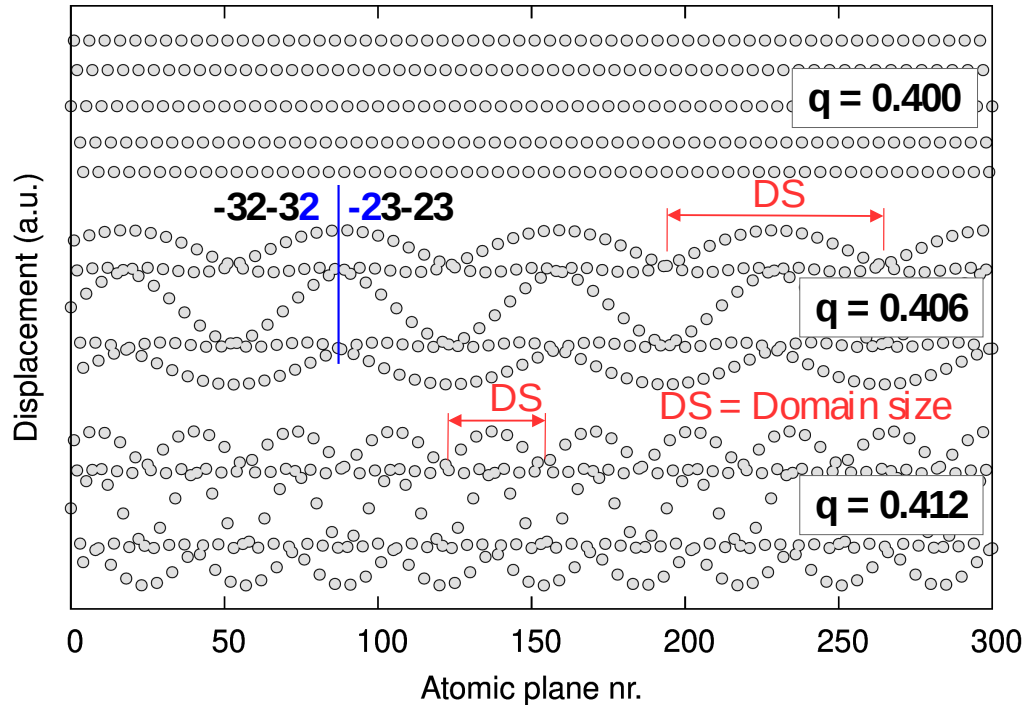
Aperiodicity – study by high-resolution q-scan



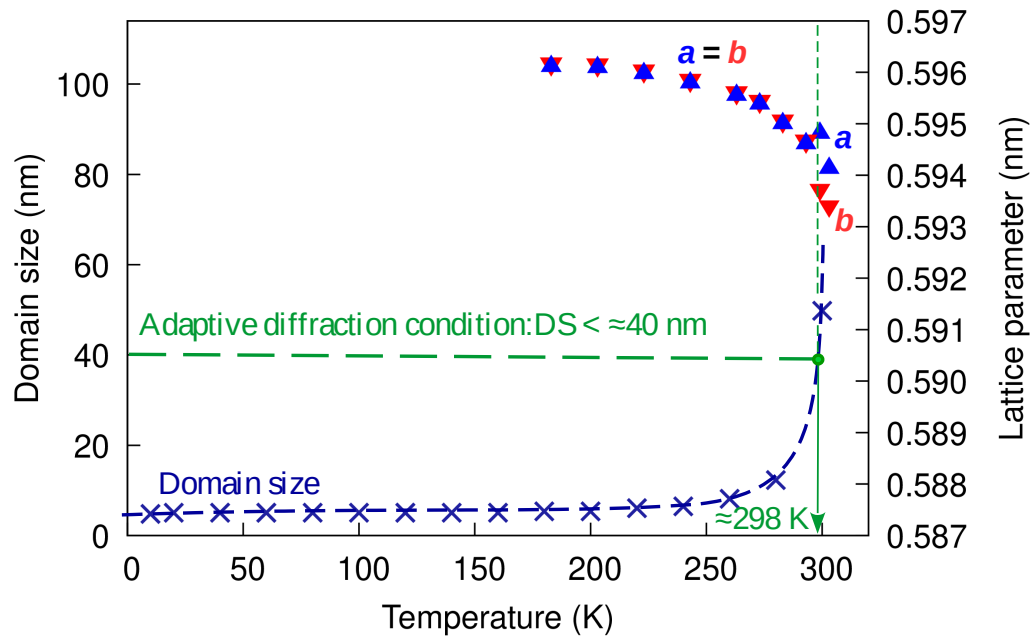
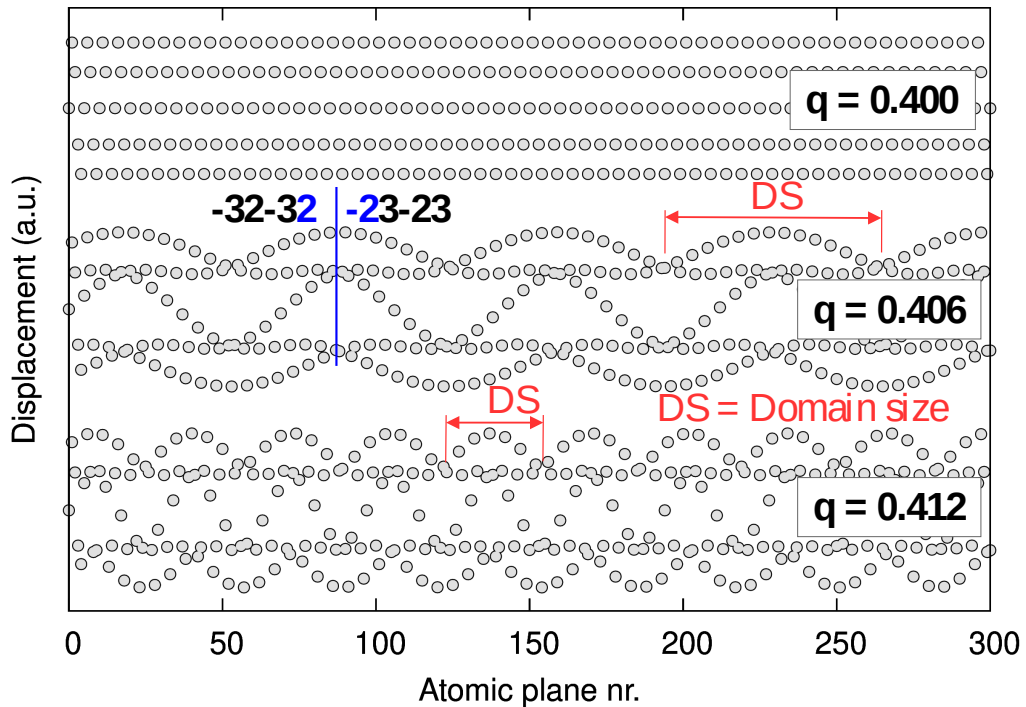
Aperiodicity – study by high-resolution q-scan



Aperiodicity results in a/b nanotwinning (!!!)

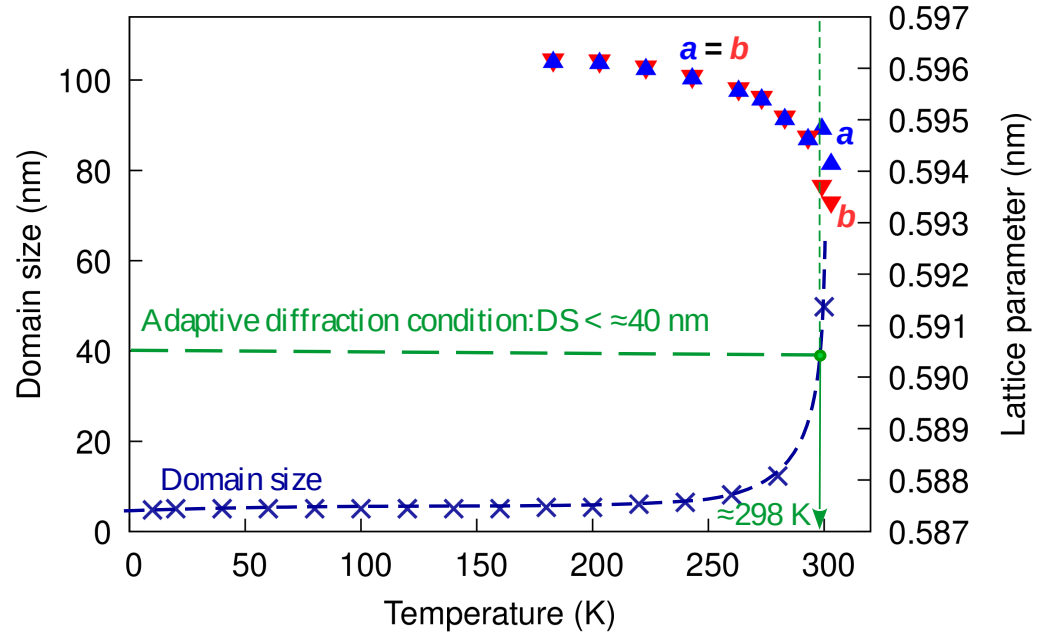
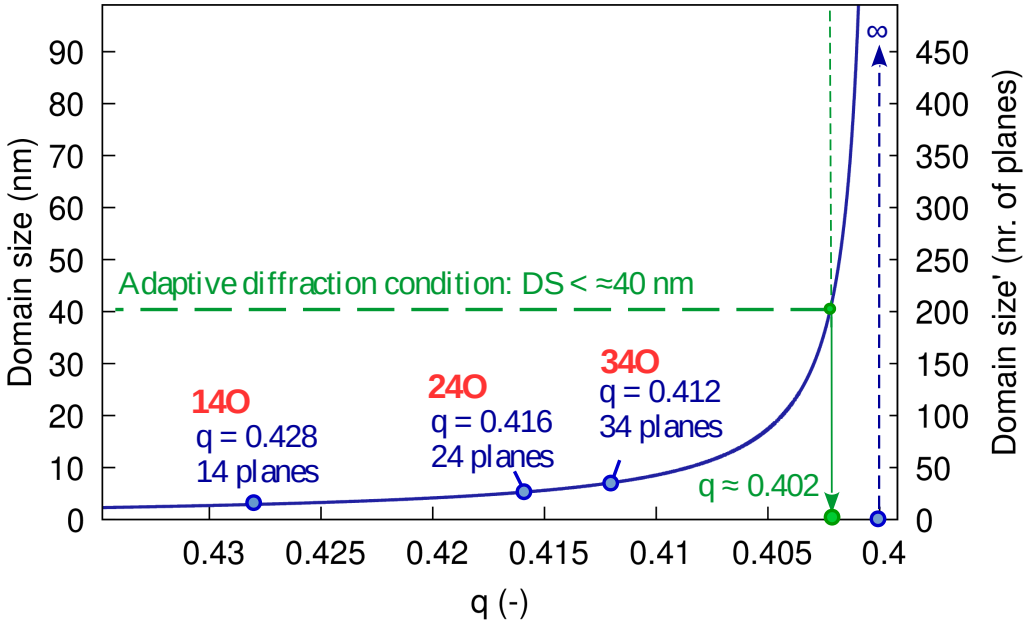


Aperiodicity results in a/b nanotwinning (!!!)



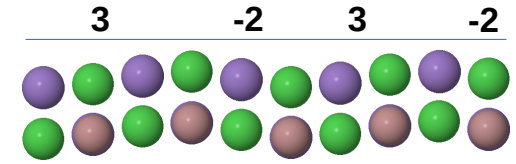
Aperiodicity results in a/b nanotwinning (!!!)

10M commens
 $q=0.4, \infty$ planes

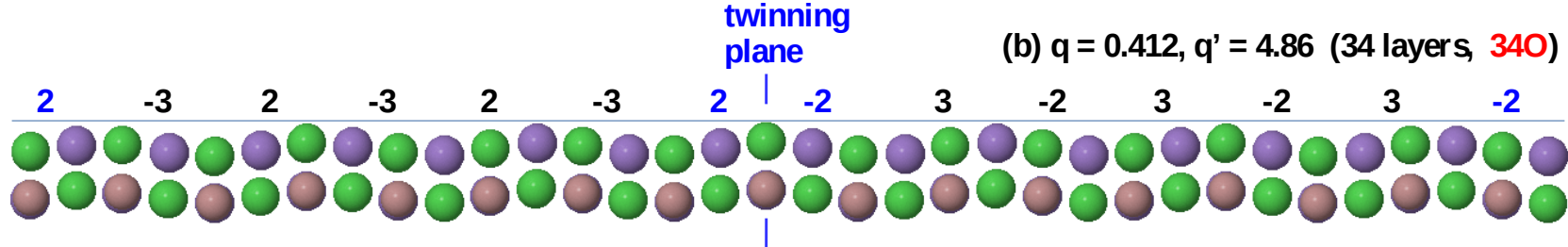


Distinct identified nanotwins/structures

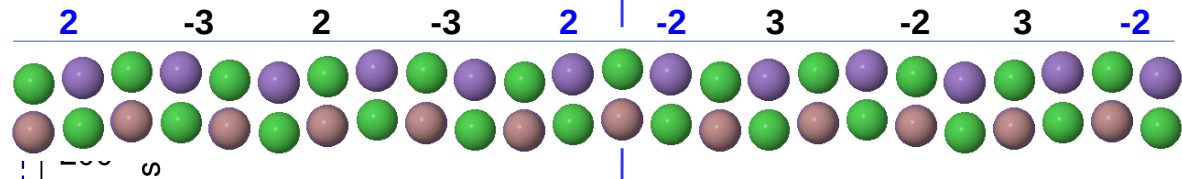
(a) $q = 0.400, q' = 5.00$ (10M commensurate)



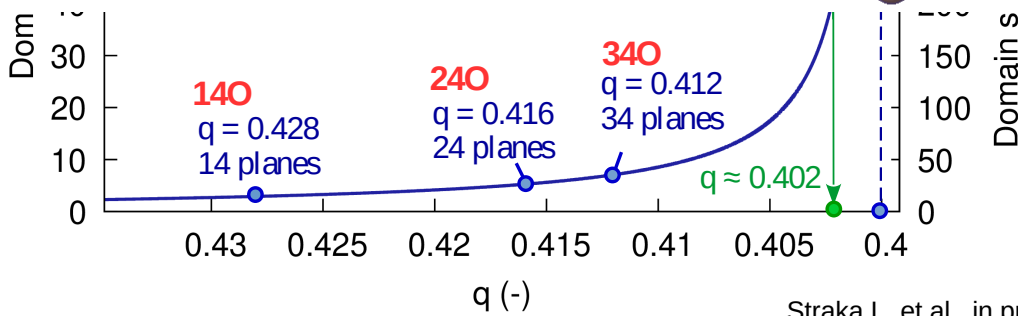
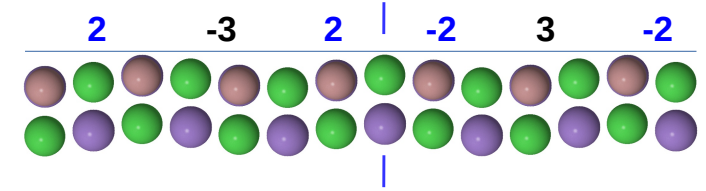
(b) $q = 0.412, q' = 4.86$ (34 layers, 340)



(c) $q = 0.416, q' = 4.80$ (24 layers, 240)

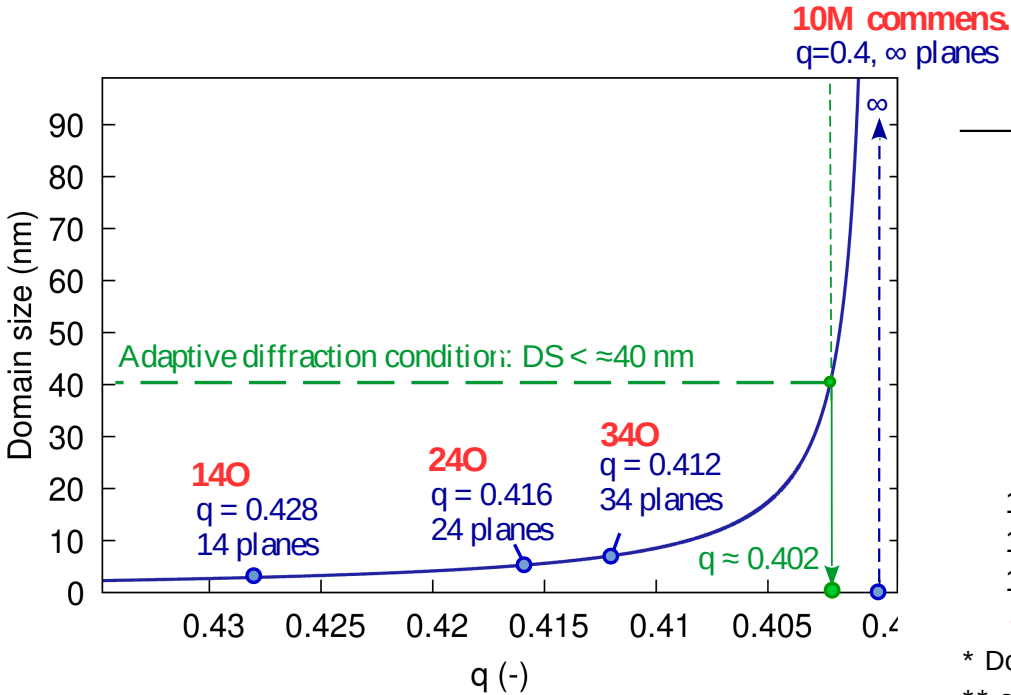


(d) $q = 3/7$ (0.428), $q' = 4.70$ (14 layers, 140)



Straka L. et al., in preparation

Distinct identified nanotwins/structures



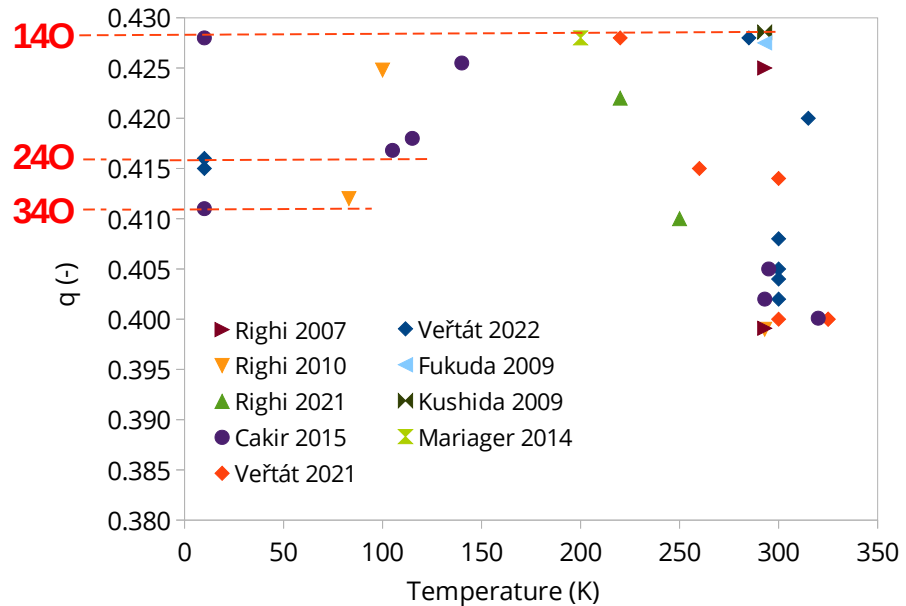
N	q' (planes)	q (-)	Domain size (planes)	Domain size (nm)	Marking
-					-
1	4.000	0.5000	4	0.8	40
2	4.500	0.4444	9	1.9	180*
3	4.667	0.4286	14	2.9	140
4	4.750	0.4211	38	8.0	380*
5	4.800	0.4167	24	5.0	240
6	4.833	0.4138	58	12.2	580*
7	4.857	0.4118	34	7.1	340
8	4.875	0.4103	78	16.4	780*
9	4.889	0.4091	44	9.2	440
10	4.900	0.4082	98	20.6	980*
11	4.909	0.4074	54	11.3	540
12	4.917	0.4068	118	24.8	1180*
∞	5.000	0.4000	∞	∞	10M comm.**

* Double cell size to comply with the L₂₁ order.

** also marked as 5M when neglecting ordering.

Distinct identified nanotwins/structures as low energy/low temperature states

Hypothesis yet to be tested: q converges to one of the nanotwinned states



N	q' (planes)	q (-)	Domain size (planes)	Domain size (nm)	Marking
-					-
1	4.000	0.5000	4	0.8	40
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11	4.909	0.4074	54	11.3	540
12	4.917	0.4068	118	24.8	1180*
∞	5.000	0.4000	∞	∞	10M comm.**

* Double cell size to comply with the L_{21} order.

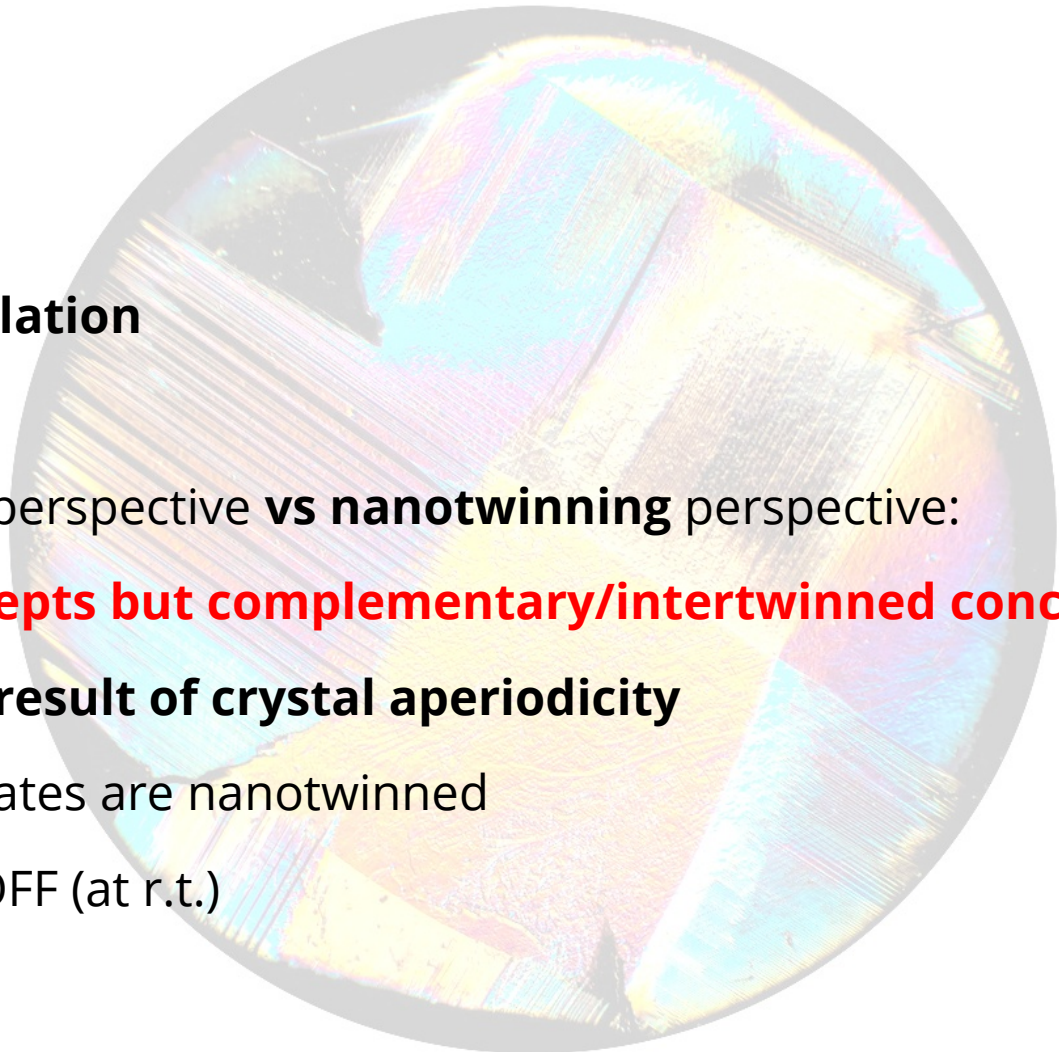
** also marked as 5M when neglecting ordering.

Summary IV

Aperiodic crystal Anharmonic modulation

Wave modulation perspective **vs nanotwinning** perspective:

- **not exclusive concepts but complementary/intertwined concepts in Ni-Mn-Ga**
- **nanotwinning is a result of crystal aperiodicity**
- Low temperature states are nanotwinned
- Nanotwinning ON/OFF (at r.t.)



Summary

Magnetic shape memory (Ni-Mn-Ga)

- very interesting at all scales
- magnetism important but (micro)structure critical for MSM functionality
- **a great platform for**
 - magnetoelastic and magnetomechanical effects (up to 12% deformation in mag. field)
 - martensite crystallography (deeply hierarchical martensite)
 - nanotwinning and aperiodic crystal concepts (**nanotwins on/of, aperiodicity on/off**)
- major **future** tasks: alternatives & applications



