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How to compute the twin index

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A few preliminary definitions

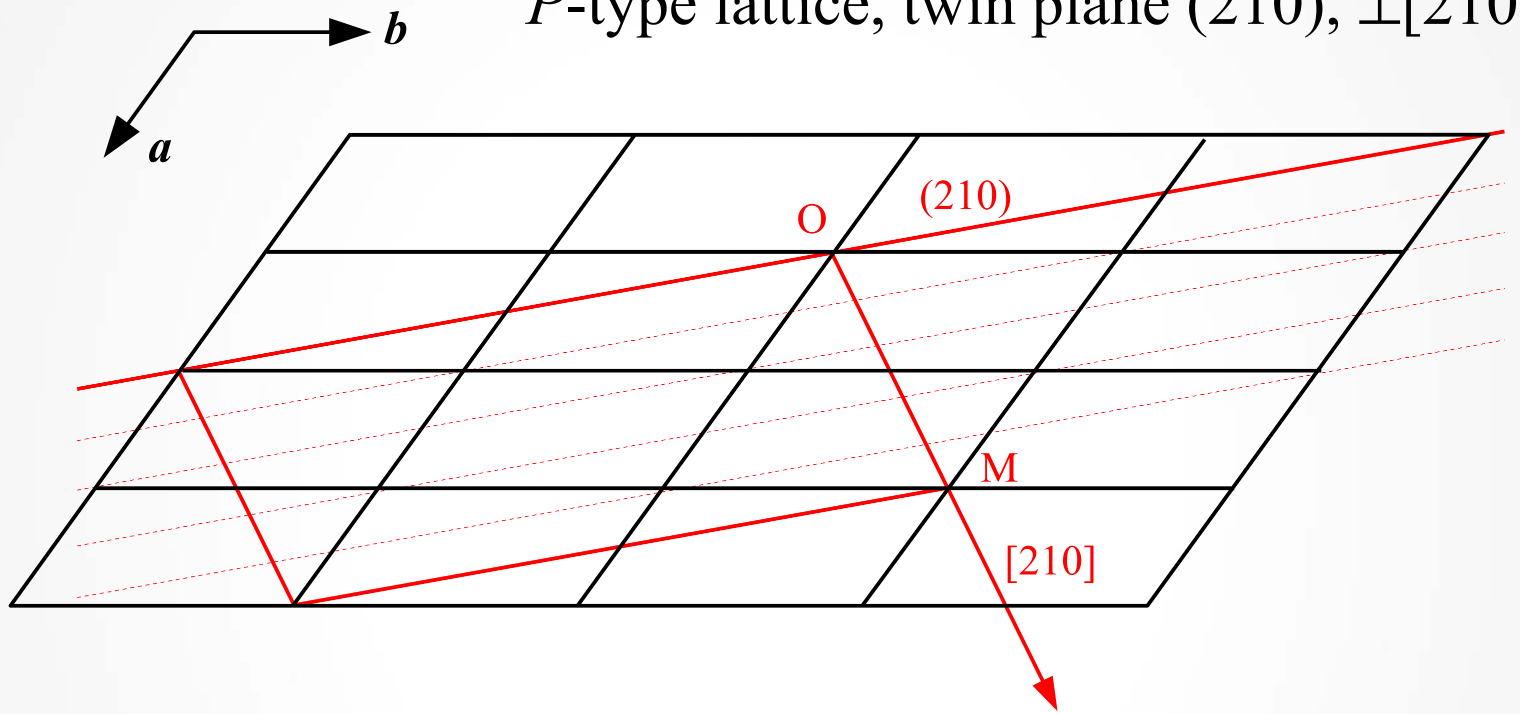
- **Twofold twins** are twins where only twin elements of order 2 exist (twofold twin axes, twin planes, twin inversion centers)
  - **First-degree twofold twins** or **binary twins** are twins where only one twin element of order 2 exists
  - **higher-degree twofold twins** are twins where more than one twin element of order 2 exist
- **Manifold twins** are twins where at least one twin element of order higher than 2 exists
  - **First-degree manifold twins** are twins where only one twin element of order higher than 2 exists
  - **higher-degree manifold twins** are twins where more than one twin element exist, of which at least one has order higher than 2

Twin index for twofold twins

A few preliminary definitions (continued)

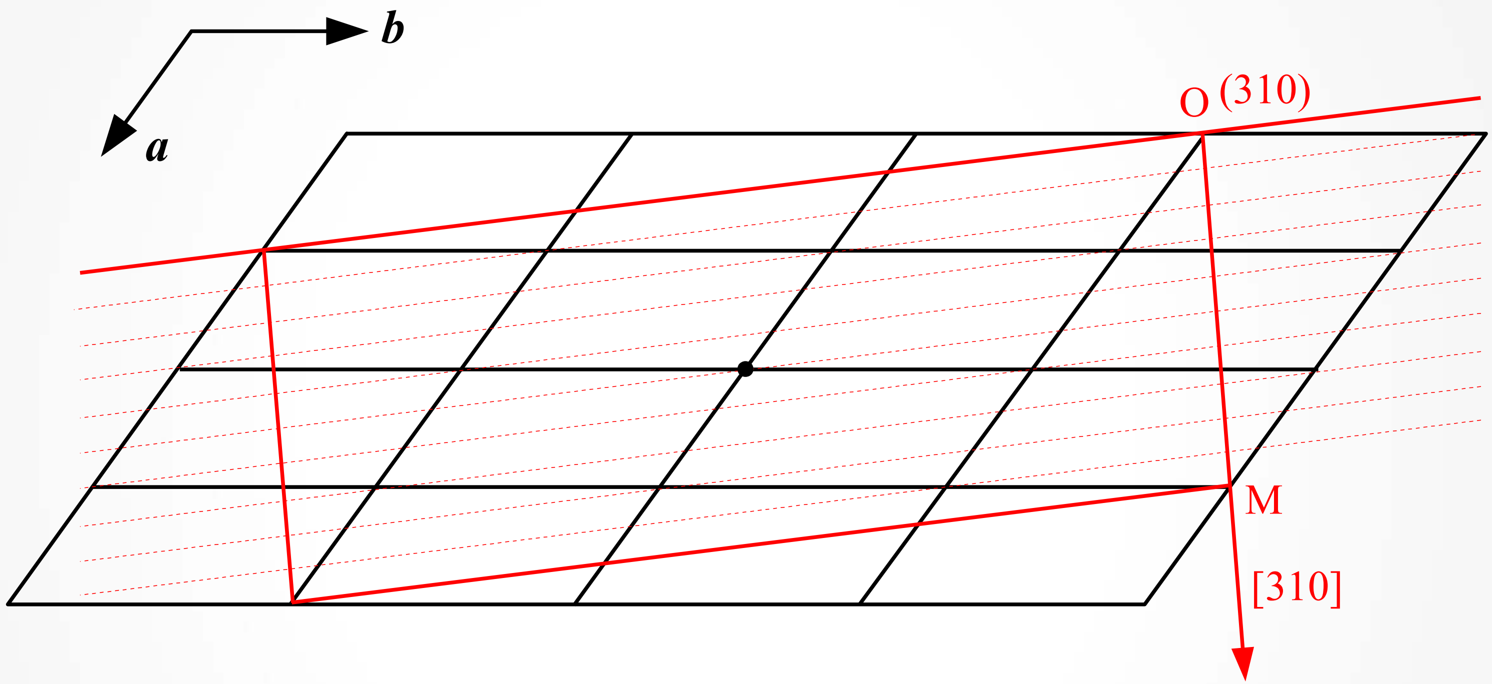
(*hkl*) and [*uvw*] are the lattice plane and lattice row defining the cell of the twin lattice
O and M are successive lattice nodes along [*uvw*]
N = number of lattice planes of the family (*hkl*) from O to M
$X = |hu+kv+lw|$
n = twin index
$\mathbf{L}_{ind}$ is the lattice of the individual
$\mathbf{L}_{T}$ is the twin lattice

P-type lattice, twin plane (210), ⊥[210]



Only nodes at the corners of the red cell are restored.
There are $N = 5$ planes of the family (210) from O to M.
$X = 2 \cdot 2 + 1 \cdot 1 + 0 \cdot 0 = 5$
The twin index is $n = 5$ ($n = N = X$)

P-type lattice, twin plane (310), ⊥[310]

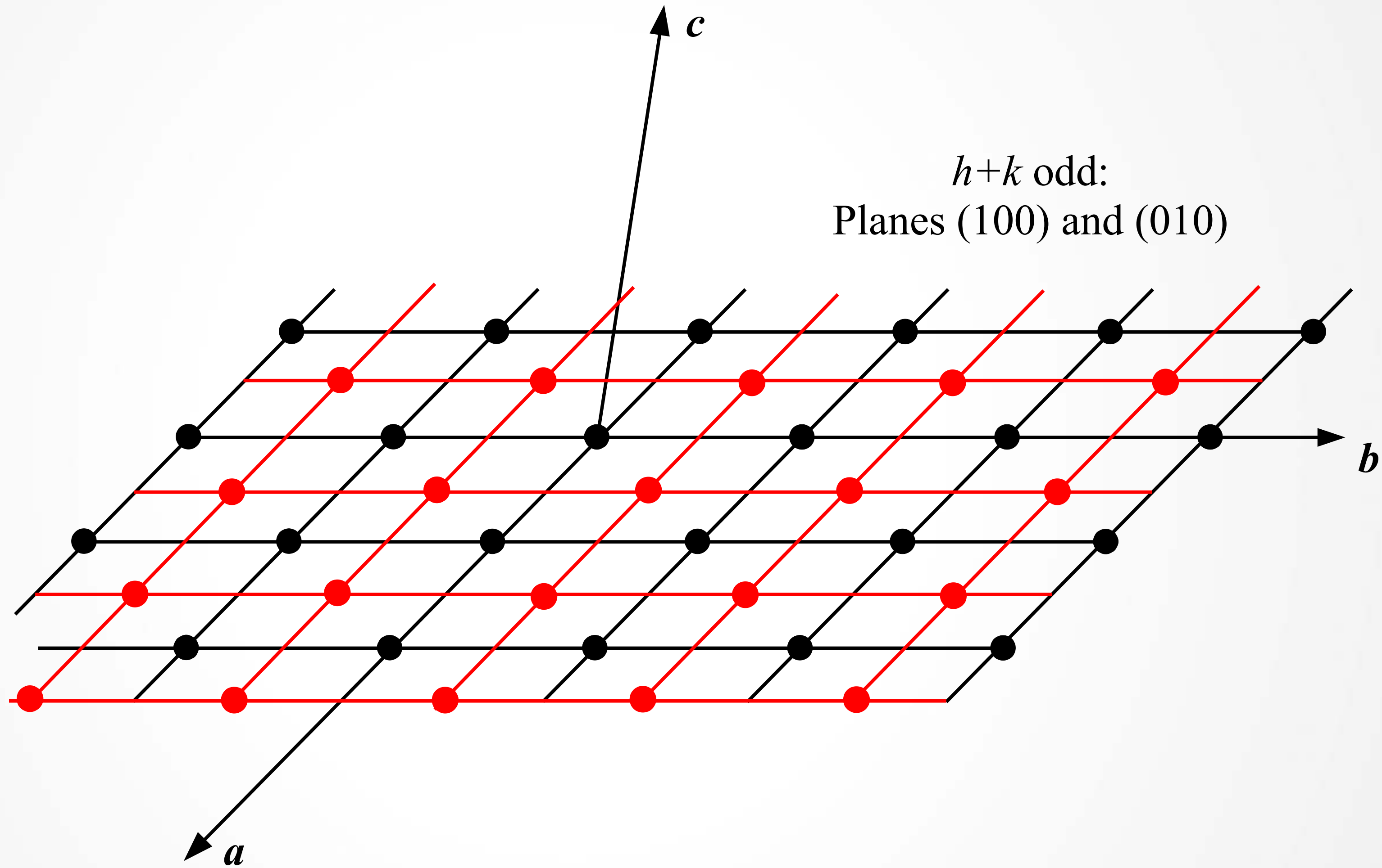


The nodes at the corners of the red cell and the node at the center are restored

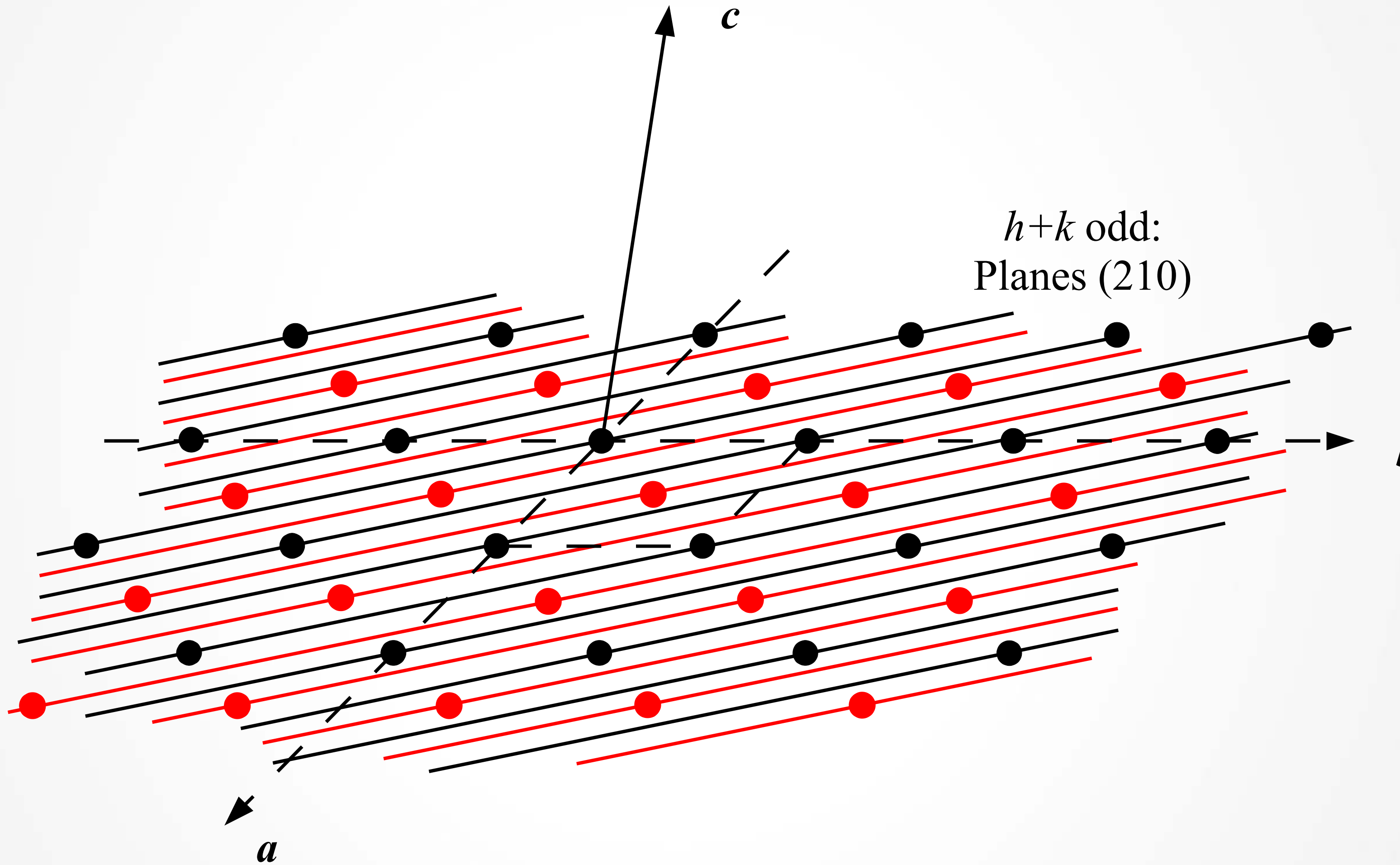
There are $N = 10$ planes of the family (310) between O and M.

$X = 3\cdot3+1\cdot1+0\cdot0=10$

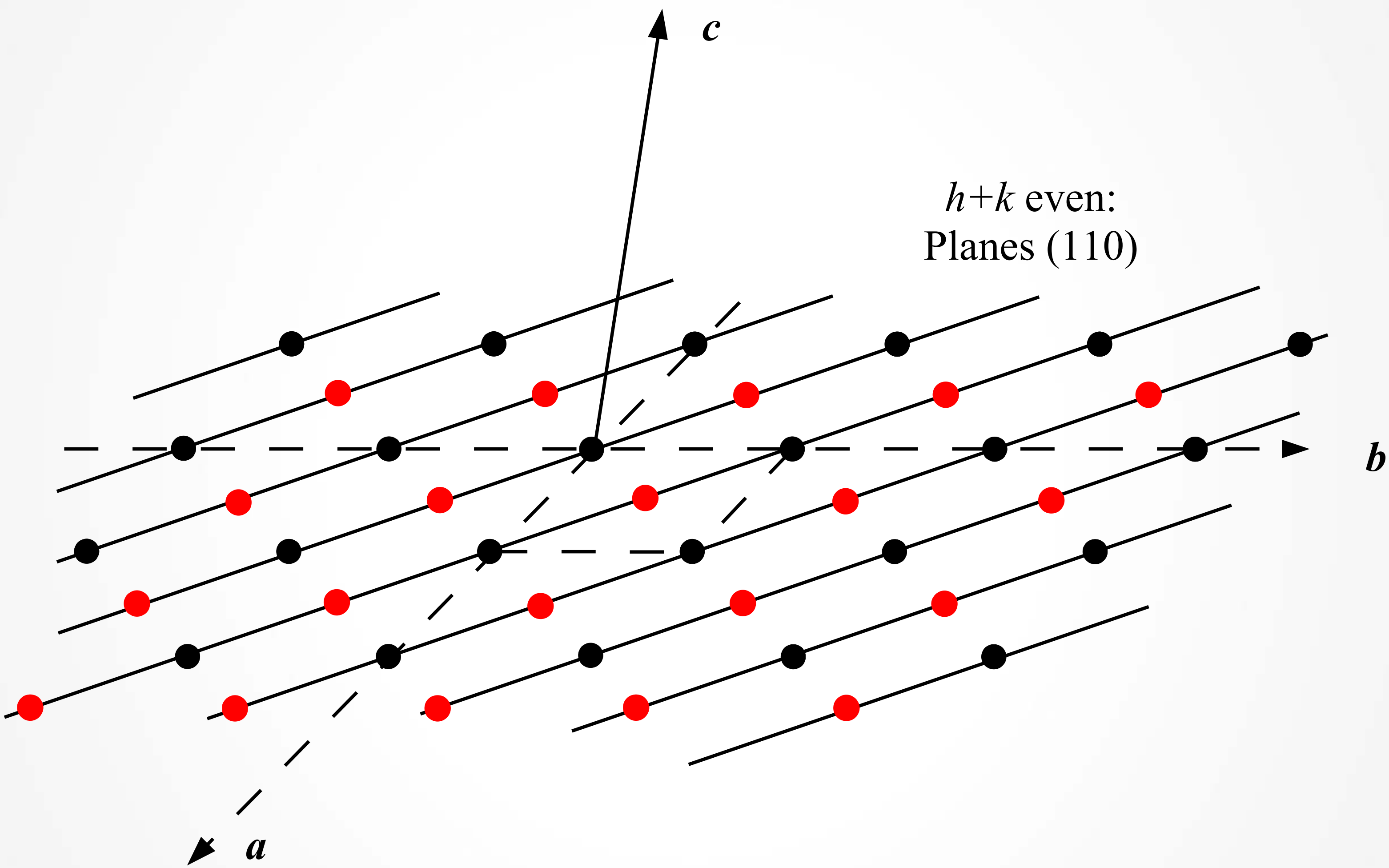
The twin index is $n = 5$ ($n = N/2 = X/2$)



Switching from *P* to *C* cell has no effect on the density of nodes on each plane but halves the interplanar distance



Switching from *P* to *C* cell has no effect on the density of nodes on each plane but halves the interplanar distance



Switching from *P* to *C* cell doubles the density of nodes on each plane but has no effect on the interplanar distance

We discover that...

(hkl) and [uvw] are the lattice plane and lattice row defining the cell of the twin lattice

O and M are successive lattice nodes along [uvw]

N = number of lattice planes of the family (hkl) from O to M

$X = |hu+kv+lw|$

n = twin index

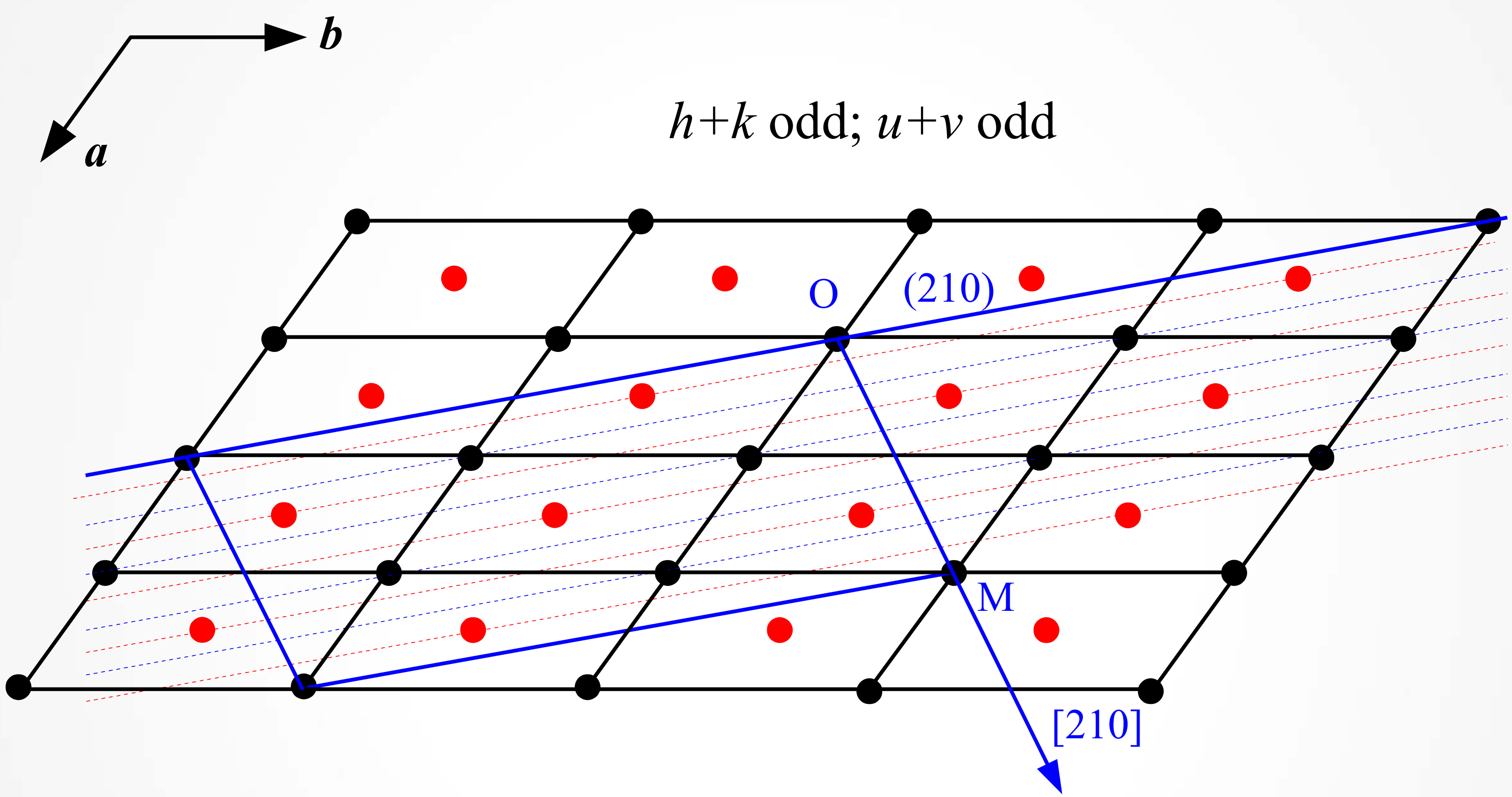
$\mathbf{L}_{ind}$ is the lattice of the individual

$\mathbf{L}_{T}$ is the twin lattice

For twofold twins, the two-dimensional coincidence index is either 1 or 0

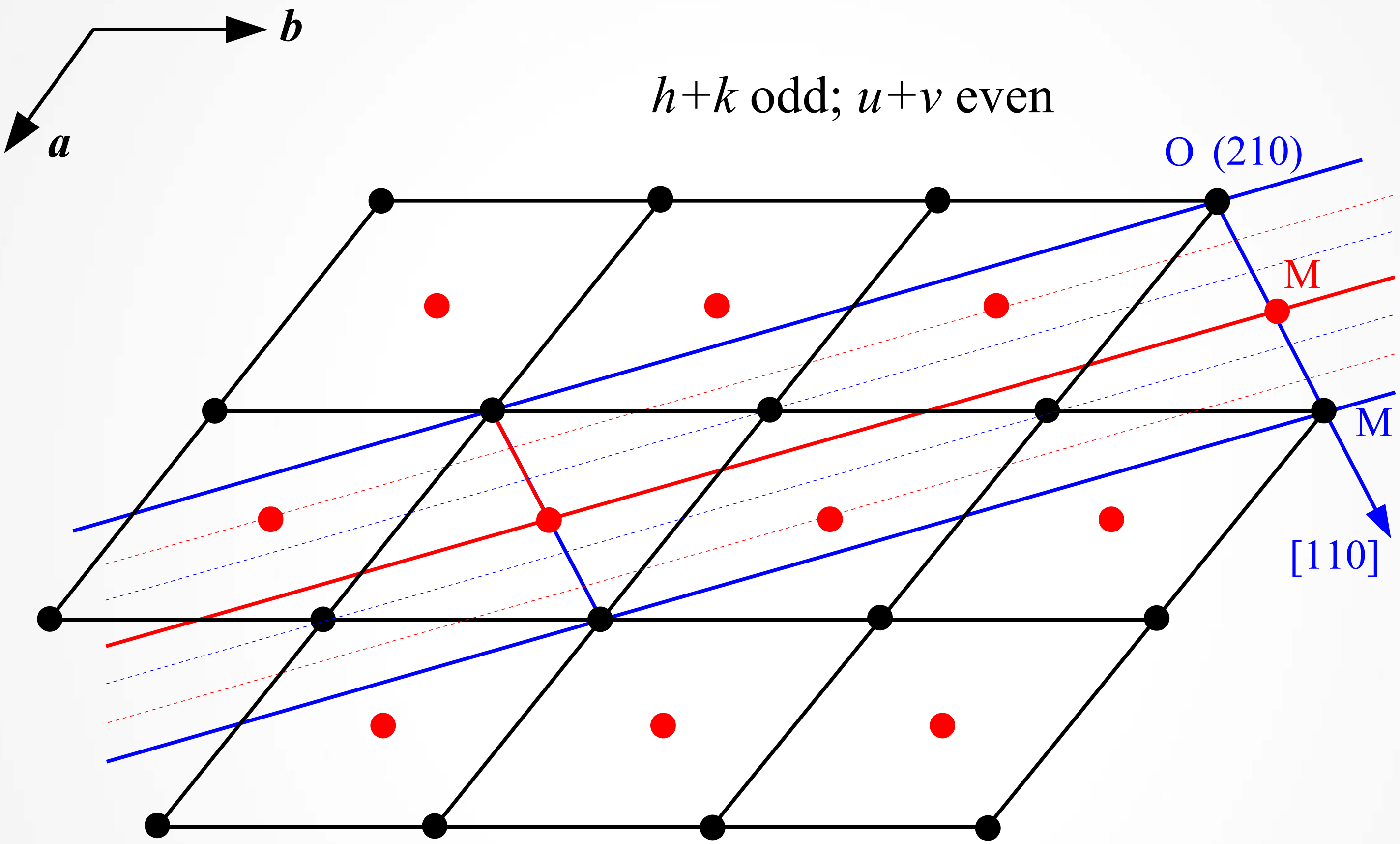
Let f be the number of lattice planes of the (hkl) family between O and M whose two dimensional coincidence index is 1

The twin index of twofold twins is simply $n = N/f$



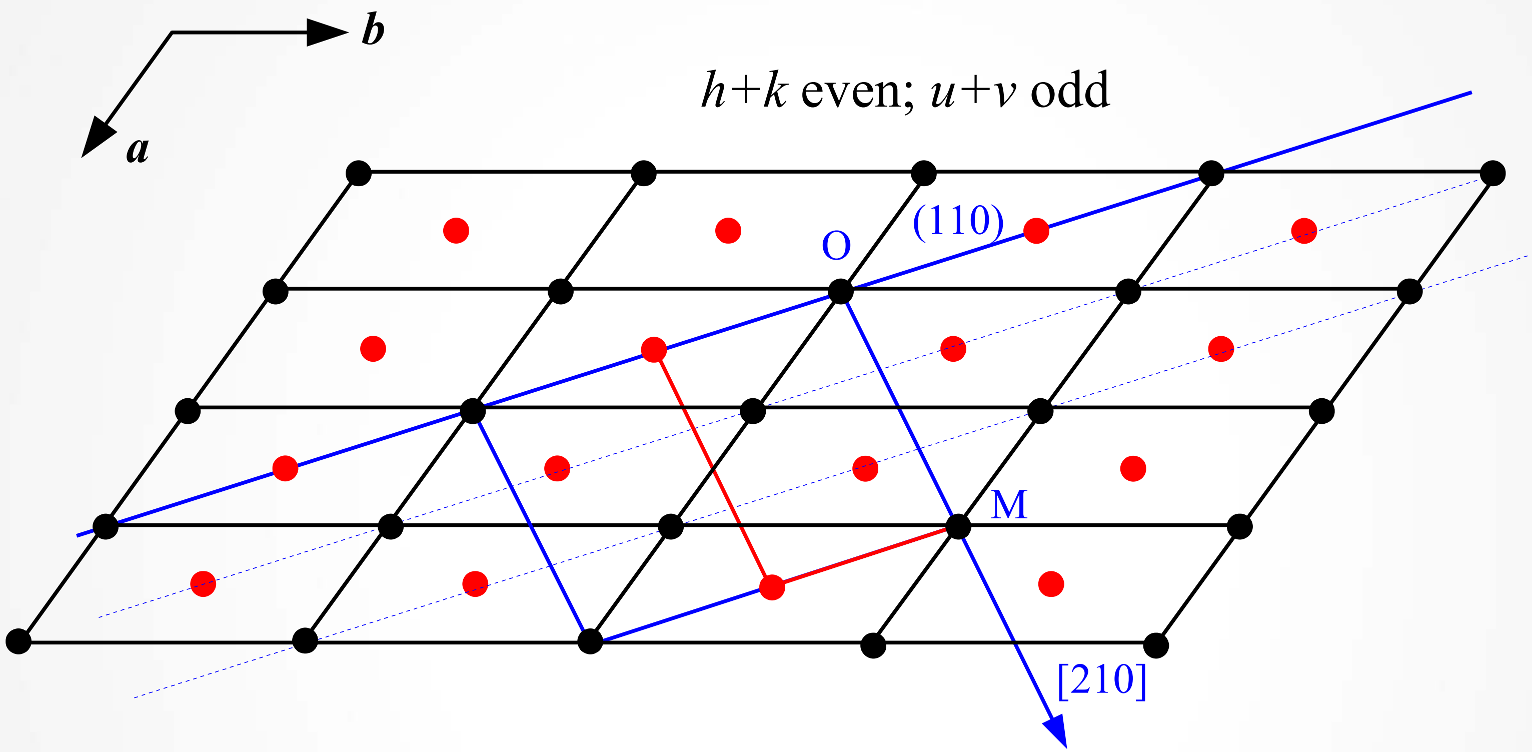
P type $\mathbf{L}_{\text{ind}}$: $N = n = X = 5$, the cell of $\mathbf{L}_{\text{T}}$ is primitive

C type $\mathbf{L}_{\text{ind}}$: $N = 2X = 10$, $n = N/2 = X = 5$, the cell of $\mathbf{L}_{\text{T}}$ is C-centered



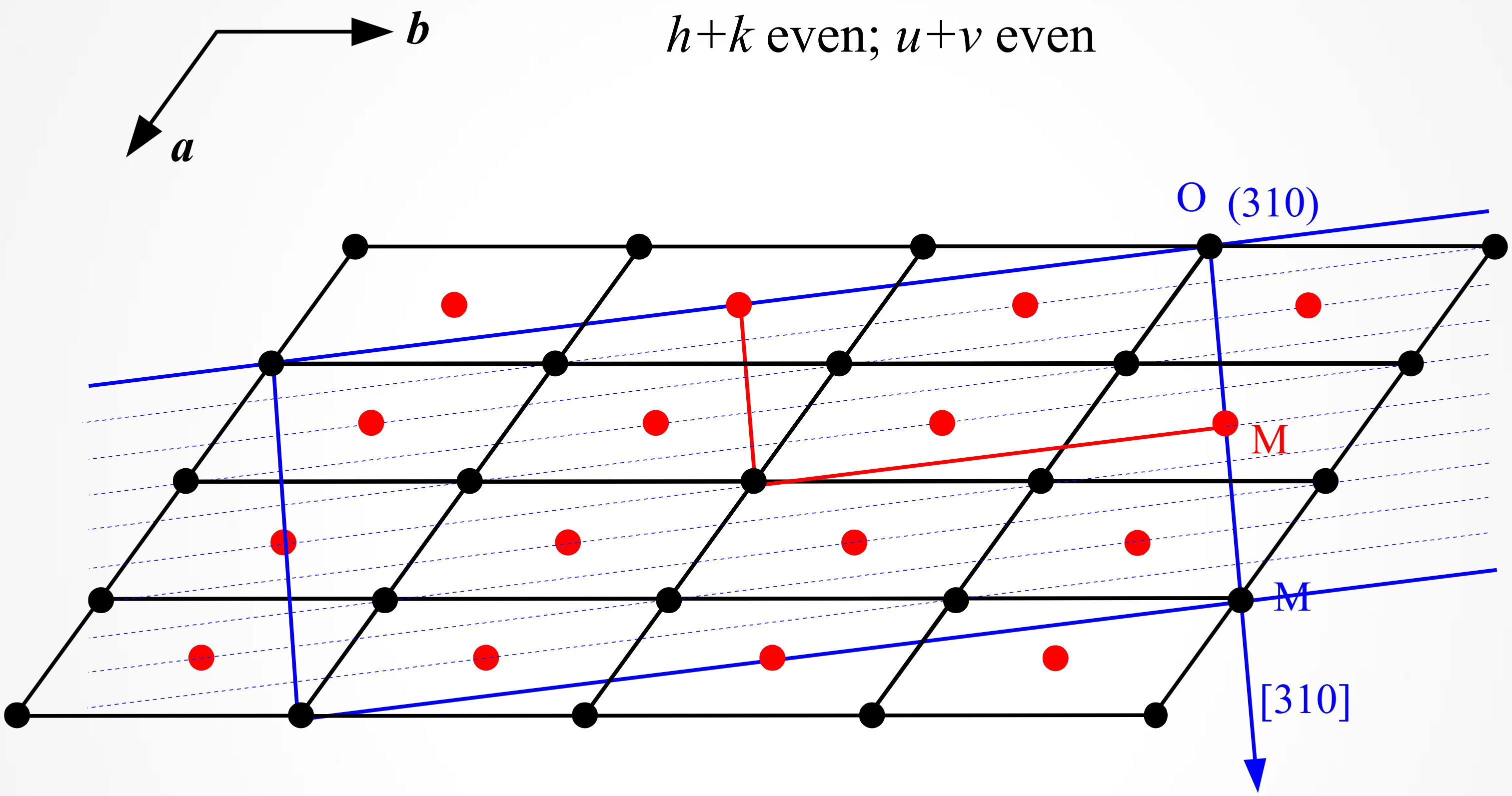
P type $\mathbf{L}_{ind}$: $N = n = X = 3$, the cell of $\mathbf{L}_T$ is primitive

C type $\mathbf{L}_{ind}$: $N = n = X = 3$, the cell of $\mathbf{L}_T$ is primitive and is twice smaller that that of *P* type $\mathbf{L}_{ind}$



P type $\mathbf{L}_{\text{ind}}$: $N = n = X = 3$, the cell of $\mathbf{L}_{\text{T}}$ is primitive

C type $\mathbf{L}_{\text{ind}}$: $N = n = X = 3$, the cell of $\mathbf{L}_{\text{T}}$ is primitive and is twice smaller that that of P type $\mathbf{L}_{\text{ind}}$



P type $\mathbf{L}_{\mathrm{ind}}$: $N = X = 10$, $n = X/2 = 5$; the cell of $\mathbf{L}_\mathrm{T}$ is C-centered

C type $\mathbf{L}_{\mathrm{ind}}$: $N = n = X/2 = 5$, the cell of $\mathbf{L}_\mathrm{T}$ is primitive and is twice smaller that that of P type $\mathbf{L}_{\mathrm{ind}}$

Summarizing....

Computation of the twin index for twofold twins

- N = number of lattice planes of the family (hkl) between two successive lattice nodes along [uvw]
- n = twin index

Primitive cell

Conditions on ***h*,*k*,*l***	Conditions on ***u*,*v*,*w***	***N***	***n***
none	none	X	if X is odd: $n = X$
			if X is even: $n = X/2$

C-centered cell

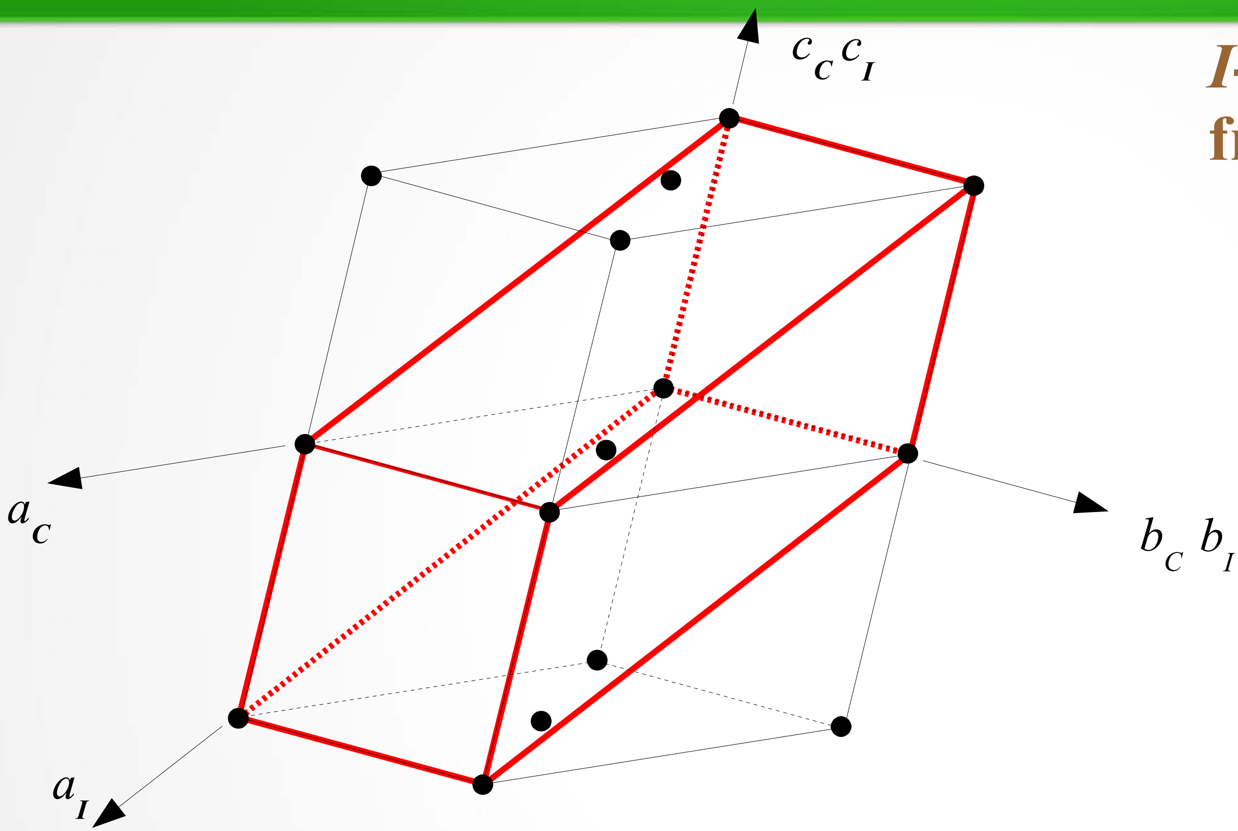
Conditions on ***h*,*k*,*l***	Conditions on ***u*,*v*,*w***	***N***	***n***
$h+k$ odd	$u+v$ and w not both even	$2X$	$n = X$
	$u+v$ and w both even	X	$n = X$
$h+k$ even	$u+v$ and w not both even	X	X odd: $n = X$
			X even: $n = X/2$
	$u+v$ and w both even	$X/2$	$X/2$ odd: $n = X/2$
			$X/2$ even: $n = X/4$

B-centered cell

Conditions on h,k,l	Conditions on u,v,w	N	n
$h+l$ odd	$u+w$ and v not both even	$2X$	$n = X$
	u+w and v both even	X	$n = X$
$h+l$ even	u+w and v not both even	X	X odd: $n = X$
			X even: $n = X/2$
	$u+w$ and v both even	$X/2$	$X/2$ odd: $n = X/2$
			$X/2$ even: $n = X/4$

A-centered cell

Conditions on h,k,l	Conditions on u,v,w	N	n
$k+l$ odd	$v+w$ and u not both even	$2X$	$n = X$
	v+w and u both even	X	$n = X$
$k+l$ even	v+w and u not both even	X	X odd: $n = X$
			X even: $n = X/2$
	$v+w$ and u both even	$X/2$	$X/2$ odd: $n = X/2$
			$X/2$ even: $n = X/4$



I-centered cell from a *C*-centered cell

Conditions on ***h,k,l***	Conditions on ***u,v,w***	***N***	***n***
$h+k+l$ odd	u, v, w not all odd	$2X$	$n = X$
	u, v, w all odd	X	$n = X$
$h+k+l$ even	u, v, w not all odd	X	X odd: $n = X$
			X even: $n = X/2$
	u, v, w all odd	$X/2$	$X/2$ odd: $n = X/2$
			$X/2$ even: $n = X/4$

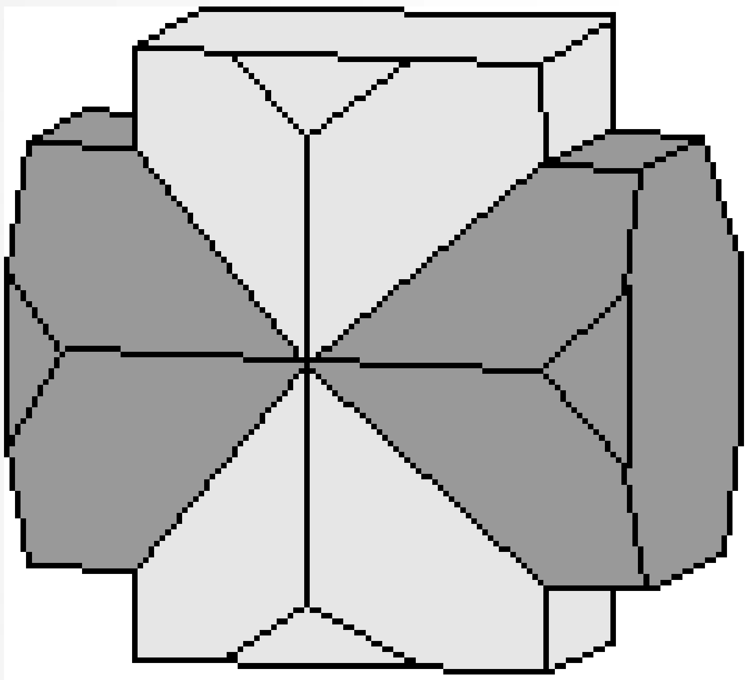
F-centered cell

F and *I* lattice types are one the dual of the other. The conditions for an *I*-centered cell apply also to an *F*-centered cell provided that (*hkl*) and [*uvw*] are exchanged.

Conditions on *h*,*k*,*l*	**Conditions on *u*,*v*,*w***	***N***	***n***
h, k, l not all odd	$u+v+w$ odd	$2X$	$n = X$
h, k, l all odd	u, v, w all odd	X	$n = X$
h, k, l not all odd	$u+v+w$ even	X	X odd: $n = X$
			X even: $n = X/2$
h, k, l all odd		$X/2$	$X/2$ odd: $n = X/2$
			$X/2$ even: $n = X/4$

What about manifold twins?

Greek-cross fourfold-twin in staurolite



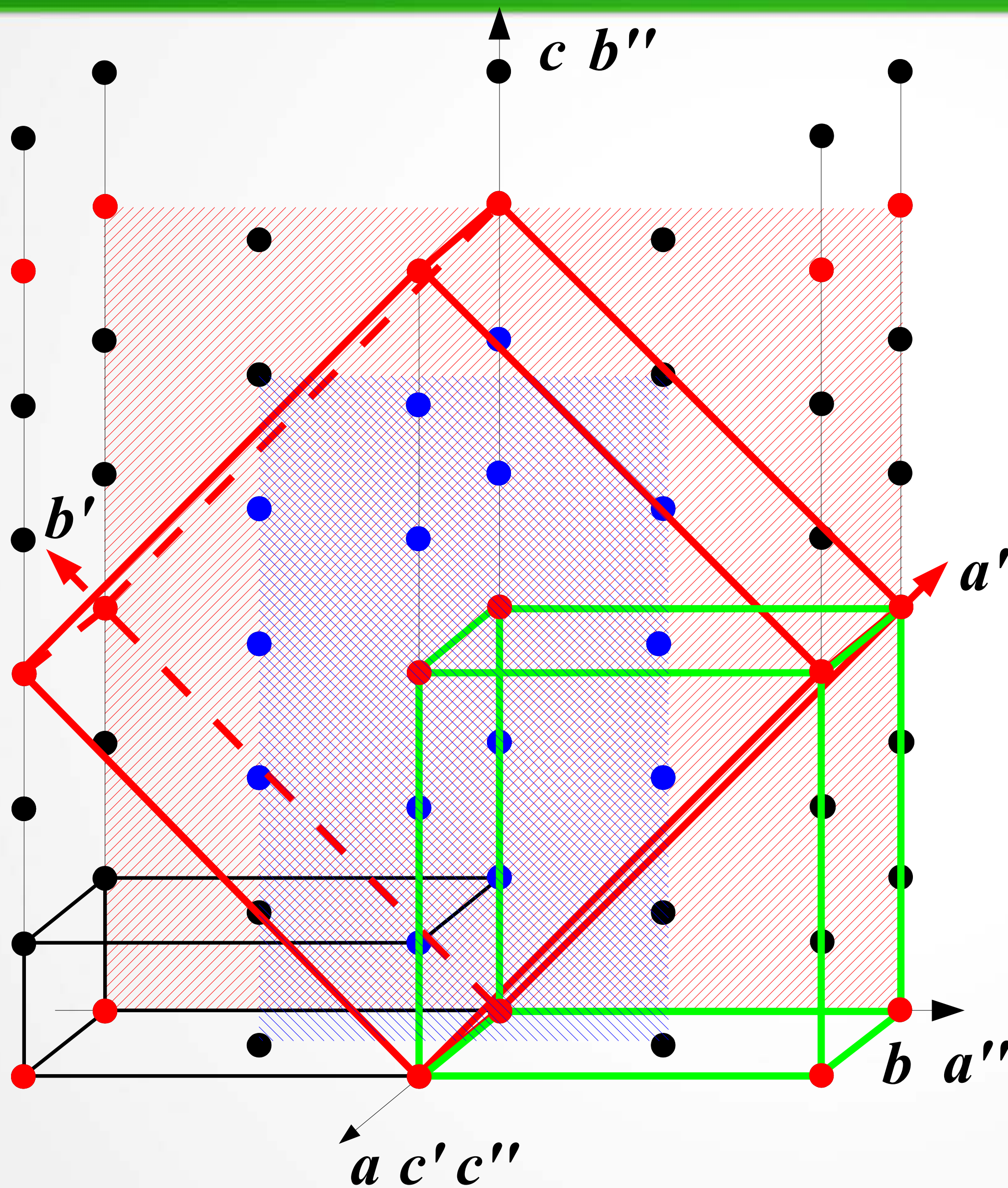
$C2/m$
$a = 7.871$ Å
$b = 16.620$ Å
$c = 5.656$ Å
$\beta = 90°$

Twin operation: $4_{[100]}$

[100] is perpendicular to (100)

$X = |1 \cdot 1 + 0 \cdot 0 + 0 \cdot 0|$

Is the twin index 1?



$n = 2 \cdot 3 \;/\; 1 = 6$

12 nodes in the tC cell of $\mathbf{L}_T$: the twin index is 6

tC is not a standard cell – let us transform it to the standard tP cell

6 nodes in the tP cell of $\mathbf{L}_T$: the twin index is 6

no nodes at all restored on this plane

2 nodes out of 6 restored on this plane (restoration index is 3)

1 plane of the (100) family out of 2 has a coincidence index of 3

How to compute the twin index of a manifold twin?

- Let N be the number of lattice planes of the (hkl) family passing within the cell of the twin lattice.
- Out of these N planes, ξ be the number of planes that are partially restored by the twin operation (the other N-ξ are not restored at all).
- Let Ξ be the reciprocal of the two-dimensional coincidence index for a plane of the (hkl) family that is partially restored by the twin operation

The twin index is $n = N\Xi/\xi$

Cumbersome? Than take a shorter route:

Find a twofold operation in the same coset and apply the classical formula!