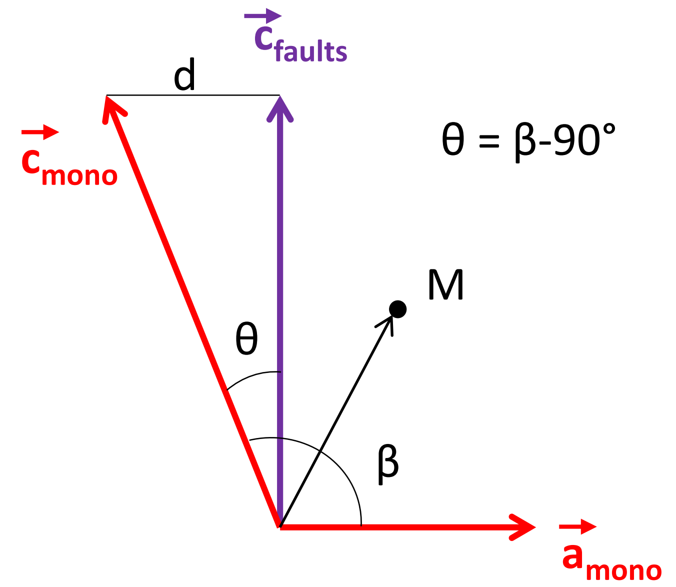
Transformation of a monoclinic cell into a FAULTS cell



$\theta = \beta - 90°$

Norms of the vectors:

$a_{faults} = a_{mono} = a$

$c_{faults} = c_{mono} * \cos(\theta) = c_{mono} * \cos(\beta - 90°)$

$d = c_{mono} * \sin(\theta) = c_{mono} * \sin(\beta - 90°)$

Vectors:

$\vec{a}_{mono} = \vec{a}_{faults}$

$\vec{c}_{faults} = \vec{c}_{mono} + (d/a).\vec{a}_{mono}$

$= \vec{c}_{mono} + (c_{mono} * \sin(\theta)/a).\vec{a}_{mono}$

Position $M(x_{faults}; z_{faults}) = M(x_{mono}; z_{mono})$

$$\mathbf{OM} = x_{mono}.\ \vec{a}_{mono} + z_{mono}.\ \vec{c}_{mono}$$

and

$$\begin{aligned}\mathbf{OM} &= x_{faults}.\ \vec{a}_{faults} + z_{faults}.\ \vec{c}_{faults} \\ &= x_{faults}.\ \vec{a}_{mono} + z_{faults}.\ (\vec{c}_{mono} + (c_{mono} * \sin(\theta)/a).\vec{a}_{mono}) \\ &= [x_{faults} + z_{faults}.(c_{mono} * \sin(\theta)/a)].\vec{a}_{mono} + z_{faults}.\ \vec{c}_{mono}\end{aligned}$$

So
$$x_{mono} = x_{faults} + z_{faults}.(c_{mono} * \sin(\theta)/a)$$
$$z_{mono} = z_{faults}$$

or:
$$\boxed{\begin{aligned} x_{faults} &= x_{mono} - z_{faults}.c_{mono} * \sin(\beta - 90°)/a \\ z_{faults} &= z_{mono}\end{aligned}}$$

Note that when starting from a triclinic cell, one should calculate c_{faults} from β and α , as well as the x_{faults} and y_{faults} atomic positions