NSXTool Internal Documentation: Notes on Literature

the NSXTool collaboration

(Dated: internal notes, work in progress, do not circulate, May 6, 2019)

I. KABSCH 2010B

Paper on "Integration, scaling, space-group assignement and post-refinement" [?].

A. Notation correspondences

	Kabsch	we
incident wavevector	$\mathbf{S}_0$	$\mathbf{k}_\mathrm{i}$
reciprocal vector	$\mathbf{p}^*$	$\mathbf{q}$
detector distance	F	?

B. Spot prediction (Sect 2.2)

This section uses vector components in the coordinate system $\{\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3\}$. In this special system, $\mathbf{p}^*$ and $\mathbf{p}_0^*$ are related to each other through a rotation by φ around vm_2, and $\mathbf{S}_0$ is perpendicular to $\mathbf{m}_1$.

1. *How to obtain* $\mathbf{p}^*$ *as function of* $\mathbf{p}_0^*, \varphi$

In $\mathbf{p}^* = D(\mathbf{m}_2, \varphi)\mathbf{p}_0^*$, just insert the standard rotation matrix D. Skip the line that involves the cross-product $\mathbf{m}_2 \times \mathbf{p}_0^*$, and directly obtain the next line.

2. *How to obtain* $\mathbf{p}^*$ *as function of* $\mathbf{p}_0^*, \mathbf{S}_0$

First, the component along $\mathbf{m}_2$: Rotation around $\mathbf{m}_2$ does not change this component, hence $\mathbf{p}^*\mathbf{m_2} = \mathbf{p}_0^*\mathbf{m}_2$.

Next, the component along $\mathbf{m}_3$: By construction, $\mathbf{m}_1 \perp \mathbf{S}_0$. This simplifies the vector product

$$\begin{aligned} \mathbf{S}_0\mathbf{p}^* &= (\mathbf{S_0}\mathbf{m}_2)(\mathbf{m}_2\mathbf{p}^*) + (\mathbf{S_0}\mathbf{m}_3)(\mathbf{m}_3\mathbf{p}^*) \\ &= (\mathbf{S_0}\mathbf{m}_2)(\mathbf{m}_2\mathbf{p}_0^*) + (\mathbf{S_0}\mathbf{m}_3)(\mathbf{m}_3\mathbf{p}^*). \end{aligned} \tag{1}$$

Insert this in the Laue equation $-2\mathbf{S}_0\mathbf{p}^* = {p_0^*}^2$, and resolve for $\mathbf{p}^*\mathbf{m}_3$.

Finally, the component along $\mathbf{m}_1$: Resolve ${p_0^*}^2 = \sum(\mathbf{p}^*\mathbf{m}_i)^2$ for $\mathbf{p}^*\mathbf{m}_1$.

3. *How to obtain* φ *as function of* $\mathbf{p}_0^*, \mathbf{p}^*$

Start from

$$\cos\varphi = \frac{\mathbf{p}^*{}_\perp \mathbf{p}_{0\perp}^*}{|\mathbf{p}^*{}_\perp| \cdot |\mathbf{p}_{0\perp}^*|} \tag{2}$$

where the subscript $\perp$ designates the projection into the plane perpendicular to $\mathbf{m_2}$.