Formulas to represent band edges in Kikuchi pattern

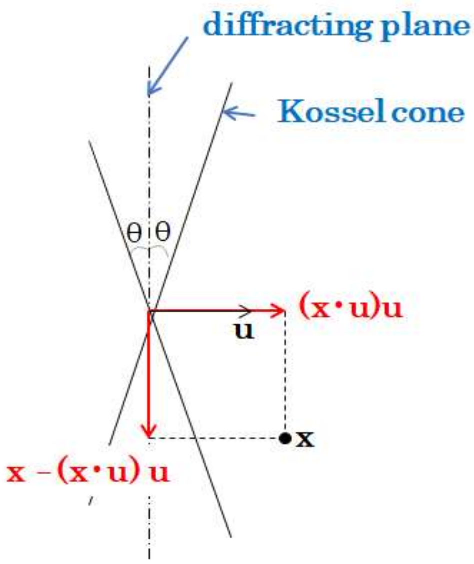
[English / Japanese]

Herein, the origin is considered as the projection center, and the axes and the unit of the length is fixed so that the phosphor screen is included in the plane z=1. The following vectors are used in the following discussion:

- $\mathbf{z} = (0, 0, 1)^T$,
- a reciprocal lattice vector $\mathbf{a}^*$,
- $\mathbf{u} = \mathbf{a}^* / |\mathbf{a}^*|$.

The band center line in a Kikuchi pattern is the intersection of the phosphor screen $\mathbf{z} \cdot \mathbf{x} = 1$ and the diffracting plane $\mathbf{a}^* \cdot \mathbf{x} = 0$. The Bragg equation $2d \sin\theta = n\lambda$ $(n = 1, 2, \ldots)$ provides the relation between the Bragg angle θ and the d-spacing $d = 1/|\mathbf{a}^*|$.

For any point $\mathbf{x}$ of the Kossel Cone as in the following figure, $(\mathbf{x} \cdot \mathbf{u})\mathbf{u}$ is the projection of $\mathbf{x}$ in the direction of $\mathbf{a}^*$, and $\mathbf{x} - (\mathbf{x} \cdot \mathbf{u})\mathbf{u}$ is the projection in the plane orthogonal to $\mathbf{a}^*$. Hence, their lengths satisfy the right-hand equality:



$$\frac{|(\mathbf{u} \cdot \mathbf{x})\mathbf{u}|^2}{|\mathbf{x} - (\mathbf{u} \cdot \mathbf{x})\mathbf{u}|^2} = \tan^2\theta.$$

Therefore, the Kossel cone is a conical surface defined by:

$$(\mathbf{u} \cdot \mathbf{x})^2 = |\mathbf{x}|^2 \sin^2\theta.$$

The band edges are the intersections of the Kossel cone and $\mathbf{z} \cdot \mathbf{x} = 1$. For simplicity, we rotate the coordinate axes of the phosphor screen, and assume $\mathbf{u} = (-\cos\sigma, 0, \sin\sigma)$. In this case, from $\mathbf{u} \cdot \mathbf{x} = 0$, the equation of the band center line is provided by:

$$x = \tan\sigma.$$

As for the equation of the band edges, we have:

$$(-x\cos\sigma + \sin\sigma)^2 = (x^2 + y^2 + 1)\sin^2\theta.$$

As a result, the band edges are represented as the following hypebola:

$$(\cos^2\sigma - \sin^2\theta)\left(x - \frac{\cos\sigma\sin\sigma}{\cos^2\sigma - \sin^2\theta}\right)^2 - (\sin^2\theta)y^2 = \frac{\cos^2\theta\sin^2\theta}{\cos^2\sigma - \sin^2\theta}.$$

The above is also equivalent to:

$$\left(\frac{\cos 2\sigma + \cos 2\theta}{\sin 2\theta}\right)^2\left(x - \frac{\sin 2\sigma}{\cos 2\sigma + \cos 2\theta}\right)^2 - \frac{\cos 2\sigma + \cos 2\theta}{2\cos^2\theta}y^2 = 1.$$

In the case of EBSD images, $\cos 2\sigma + \cos 2\theta = \cos 2\sigma + \cos 2\theta > 0$ holds. The band width equals the distance between the two intersections $\sigma_{begin}, \sigma_{end}$ of the x-axis and the band edges: Furthermore, we have:

$$\tan\sigma_{begin} = \frac{\sin 2\sigma - \sin 2\theta}{\cos 2\sigma + \cos 2\theta} = \frac{(e^{i(\sigma+\theta)} + e^{-i(\sigma+\theta)})(e^{i(\sigma-\theta)} - e^{-i(\sigma-\theta)})}{i(e^{i(\sigma+\theta)} + e^{-i(\sigma+\theta)})(e^{i(\sigma-\theta)} + e^{-i(\sigma-\theta)})} = \tan(\sigma - \theta),$$
$$\tan\sigma_{end} = \frac{\sin 2\sigma + \sin 2\theta}{\cos 2\sigma + \cos 2\theta} = \frac{(e^{i(\sigma+\theta)} - e^{-i(\sigma+\theta)})(e^{i(\sigma-\theta)} + e^{-i(\sigma-\theta)})}{i(e^{i(\sigma+\theta)} + e^{-i(\sigma+\theta)})(e^{i(\sigma-\theta)} + e^{-i(\sigma-\theta)})} = \tan(\sigma + \theta).$$

As a result, $\sigma_{begin} = \sigma - \theta$, $\sigma_{end} = \sigma + \theta$ are also obtained.

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