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ON THE GEOMETRICAL RELATIONSHIP BETWEEN KIKUCHI LINE POSITION AND EXCITATION ERROR IN ELECTRON DIFFRACTION⁺

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All of the main features of the geometry of Kikuchi lines can be thoroughly explained using the treatment first proposed by Kikuchi¹ in which the observed diffraction lines are considered to arise from the elastic (Bragg) scattering of electrons that had been previously scattered inelastically by the specimen. The positions of the lines occur at the intersection of Kikuchi cones or Kossel cones with the Ewald sphere,^{2,3} giving an accurate indication of the orientation of the specimen relative to the incident beam direction, and providing a rapid means (inspection) of deducing the sign of the deviation parameter, s . Less obvious from these traditional presentations however is the actual *magnitude* of s . This paper presents an alternative geometrical construction employing multiple Ewald spheres to illustrate the phenomenon of multiple scattering⁴ which is responsible for the formation of Kikuchi lines, and to provide a straightforward derivation of the excitation error from the relative positions of the Kikuchi lines and their corresponding diffraction spots.

The proposed construction uses the simplifying assumption that the amount of energy lost during the inelastic scattering event is negligibly small. It follows that the Ewald sphere construction for points comprising the Kikuchi lines will be identical to that for points at individual diffraction spots. Specifically, the centers of all reflecting spheres in contact with a Kikuchi line lie on a circle in the bisector plane of the corresponding scattering vector $\mathbf{g}$ (see Fig. 1). By definition, the distance between any point on this circle and the origin of reciprocal space is $|\mathbf{K}| = 1/\lambda$. Since the circle is the locus of Ewald sphere centers for a given Kikuchi line, any vector originating on this circle and passing through a reciprocal lattice point at $\mathbf{g}$ will terminate on the Kikuchi line as shown in Fig. 1.

Figure 2 is a modification of this construction to now show a finite deviation parameter, $s > 0$. In a sufficiently thin crystal, the wavevector $\mathbf{K}$ would correspond to the incident wavevector onto the specimen, and $\mathbf{K}'$ the scattered wavevector due to a Bragg event. Both of these vectors originate at point C_1 , the origin of the Ewald Sphere for this original beam incidence. For a sufficiently thick crystal, the effect of inelastic scattering would be to create a new incident direction, centering a new Ewald sphere at C_K , and producing a new scattered wavevector $\mathbf{K}_g$, which passes through the reciprocal lattice point at $\mathbf{g}$ and terminates on a Kikuchi line (c.f. Fig. 1).

To compare the geometrical relationship between $\mathbf{K}$, $\mathbf{K}'$ and $\mathbf{K}_g$, it is necessary to shift the vector $\mathbf{K}_g$ to $\mathbf{K}_g'$ such that its origin is C_1 (see Fig. 2). This operation is equivalent to giving all scattering vectors the same origin. One can then extend the scattering trajectories of those vectors to real space as shown in Fig. 2. Consequently P is the position of the forward scattered beam in real space, Q is the position of the diffracted beam, and R is a point on the Kikuchi line ($s > 0$) which corresponds to the scattering vector $\mathbf{K}_g'$. If the real space vector connecting P and Q is $\mathbf{r}$, then the excitation error can then be computed by recognizing that $\theta_1 = s/g$, and $\theta = r/L$, where L is the camera constant distance, yielding $s = rg/L$.

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Fig. 1 Geometrical construction showing the circular locus of origins of all Ewald Spheres which simultaneously pass through both the origin of reciprocal space and the reciprocal lattice point at **g**. The extension of the line connecting any point (**C**) on the circle with **g** intersects the corresponding Kikuchi line in the diffraction plane.

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Fig. 2 Schematic Reciprocal Lattice/Ewald Sphere construction showing the geometrical relationship between the excitation error ($\mathbf{s}$), the position (Q) of the Bragg diffracted spot, and a point (R) on the corresponding (excess) Kikuchi line. Point (R) is colinear with points (P) and (Q). The two Ewald Sphere segments shown here are due to two elastic scattering events, one corresponding to the incident beam which is centered at C_I , and the other corresponding to the direction resulting from an inelastic scattering event, which is centered at C_K . This latter is responsible for the formation of Kikuchi lines. The above construction permits rapid association between the diffraction geometry of reciprocal space and the measured distances in the diffraction pattern, giving an accurate value for the magnitude of $\mathbf{s}$ (see text).

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