FURTHER COMMENTS ON MILLER INDICES, RECIPROCAL SPACE VECTORS, INTERPLANAR SPACINGS, AND PLANAR INTERCEPTS WITH THE AXES OF BRAVAIS LATTICE

From the three primitive vectors that generate the Bravais lattice, \( \vec{a}_1, \vec{a}_2, \vec{a}_3 \), one can construct the reciprocal space using the three reciprocal lattice vectors, \( \vec{b}_1, \vec{b}_2, \vec{b}_3 \), where

\[
\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)},
\]

etc. One notices that the condition

\[
\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}
\]

is satisfied in general, i.e. even when the lattice is triclinic. Every reciprocal lattice vector (not necessarily a primitive reciprocal lattice vector) defines a set of (infinite) parallel planes in the direct lattice. These direct-space planes are orthogonal to the direction of the reciprocal lattice vector, \( \vec{K} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3 \) (where \( h, k, l \) are integers), and are separated by an interplanar distance of

\[
d_{hkl} = \frac{2\pi}{|\vec{K}|}.
\]

If \( \vec{K} \) is the shortest reciprocal lattice vector in its direction, i.e. if \( h, k, l \) have no common factors, every plane in the direct space will contain an infinite number of Bravais lattice points and there will not be any Bravais lattice point that is not contained in one of these planes. If \( \vec{K} \) is not the shortest reciprocal lattice vector in its direction, then not every plane in the direct space will contain Bravais lattice points. For example, if \( \vec{K} = 3\vec{K}' \) where \( \vec{K}' \) is also a reciprocal lattice vector and is the shortest in this direction, then only one-third of the planes in direct space, as defined by \( \vec{K} \), will contain (infinite) Bravais lattice points. Notice that everything that has been discussed so far holds in general, even for triclinic lattice.

Our first task is to determine the intercepts of the \( hkl \) planes with the principal axes in direct space: \( n_1a_1, n_2a_2 \), and \( n_3a_3 \). Let one of the \( hkl \) planes pass through the origin, as shown in the figure, we want to know what the intercept of the immediate adjacent plane with the \( \vec{a}_1 \) axis is. Namely, we want to know what \( n_1 \) is. In the figure, the planes are drawn as red dashed lines and the direction of the reciprocal lattice vector \( \vec{K} \) is indicated by the black dashed line. From the figure it is clear that

\[
n_1a_1 = d_{hkl} / \cos \theta_1.
\]
Since $\theta_i$ is the angle the $\vec{a}_i$ axis makes with the vector $\vec{K}$, we can write

$$\cos \theta_i = \frac{\vec{a}_i \cdot \vec{K}}{a_i |\vec{K}|} = \frac{\vec{a}_i \cdot (h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3)}{a_i |\vec{K}|} = \frac{2\pi h}{a_i \left(\frac{2\pi}{d_{hkl}}\right)} = \frac{h d_{hkl}}{a_i}.$$  

Upon plugging into the previous equation, we get

$$n_i = 1/h.$$  

It is obvious that similar procedures will lead to

$$n_2 = 1/k, \quad n_3 = 1/l.$$  

The intercepts on the three axes are, therefore, $a_i/h, a_2/k$, and $a_3/l$, respectively. Furthermore, one notices that these results are valid in general, not just for cubic systems.

For cubic systems, the magnitude of $\vec{K} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ is simply obtained,

$$|\vec{K}| = \frac{2\pi}{a} \sqrt{h^2 + k^2 + l^2},$$

and, therefore,

$$d_{hkl} = \frac{2\pi}{|\vec{K}|} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}.$$  

The last result can be independently verified by first drawing a perpendicular line $f$ to the line segment representing the intercept of the plane with the horizontal plane. From the area of the horizontal triangle, one obtains

$$f = \frac{(a/k)(a/h)}{\sqrt{a^2/h^2 + a^2/k^2}} = \frac{a}{\sqrt{h^2 + k^2}}.$$  

Applying the same procedure to the right angle triangle, with $f$ as one of its sides, one obtains

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2}} \frac{a}{l} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}.$$