Supplementary Materials

for

Quaternion and biquaternion representations of proper and improper transformations in non-Cartesian reference systems

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1. Example: Non-symmetric rotation in the monoclinic system

A non-symmetry rotation is exemplified for the monoclinic system: the rotation of vector ***a*** by angle -β around vector ***b***, when we assume the following unit-cell parameters: *a* = *b* = 1, *c* = 2; α = γ = 90°, β ≠ 90°.



As , we have

1. Example: Rotation about reciprocal vector *cr* in the monoclinic lattice
 *a*=*b*=*c*/2, β>90°

The numerical calculations:

Thus, the rotation by 90° around ***cr*** exactly superimposes the image of vector ***a*** with vector ***b*** along axis [y] (because for this example we assumed the equal length of ***a*** and ***b***).

1. Example: Vector *a* rotated by 180° about the direction [110] for
 orthorhombic unit cell *a=b*/2=c=1 and α=β=γ=90°

First, let’s rotate vector ***r*** = [001] by angle 180° about the direction [110] for an orthorhombic lattice with unit cell *a=b*/2=c=1 and α=β=γ=90°. The multiplication rules for quaternions in this system are:

.

So, the quaternion for the requested rotation is: *q*(180°, [110]) = (*i* + *j*)/

and the rotated vector ***r’*** can be calculated as

 ***r’*** = *q****r****q*\* = [(*i* + *j*)/] *i* [–(*i* + *j*)/]=

 = (–1 – 2*k*)( *–i – j*)/5 =

 = –3*i*/5 + 2*j*/5,

which corresponds to direct-space coordinates ***r’*** = [–3/5, 2/5, 0].

1. Example: Rotation about vector [110] in the monoclinic lattice *a*=*b*/2=*c*, γ =120°

The lattice is monoclinic (non-conventional, in order to clarify comparisons to the previous example) with unit-cell parameters *a = b*/2 = c = 1, α = 90°, β = 90°, γ = 120°. Vector ***r*** = [001] is to be rotated by angle 180° about direction [110]



The quaternion multiplication rules for this system are:

The metric matrix *G* is

The length of the vector ***g1*** = [110] is

The quaternion for the rotation by angle 180° about the direction [110] is

The rotation vector ***r =*** [100] by angle 180° about the direction [110] is

Which corresponds to the crystal-lattice vector

1. Example: Rotation about vector in the monoclinic lattice *a*=*b*/2=*c*, γ =120°

The lattice and unit cell like in the example above (S4), but vector ***r*** = [100] is rotated by angle 180° about crystal direction . Hence:

The quaternion for the rotation by angle 180° about direction is

The rotation vector ***r =*** [100] by angle 180° about direction is



Thus, the rotation of ***r*** = [100] about direction by angle 180° results in vector ***r’***= .