Modelling of crystals' morphology using Formex algebra

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Abstract
The objective of this paper is to introduce an algebraic and computational method for three dimensional modelling of crystals' morphology. This method employs Formex algebra (Nooshin [4]) together with some crystallographic concepts, such as Miller indices and symmetry elements. A function called Miller function has been developed to create models of crystals. Miller function not only allows modelling of crystals but also enables creation of different habits of each crystal by changing the parameters of Miller function. Miller function has been implemented in the Formian software (Nooshin et al. [5]). This function helps designers to create their desired crystal forms. Also, some examples are shown for habits of the Rutile crystal.

Keywords: Formex Algebra, Crystal, Miller indices, Modelling, Formian.

1. Introduction
Crystals are three dimensional objects consisting of periodic ordered atoms, molecules or ions, bounded by natural plane faces. Crystals as the natural based forms can be used for the configuration of space structures. Study of crystal morphology provides a convenient basis for working on the geodesic forms and other configurations in space structures. Every crystal belongs to one of seven crystallographic systems with special lattice parameters (a, b, c, α, β and γ) (Borchardt-Ott [1]). The faces of crystal are planes which need to be defined in three dimensions. A family of lattice planes is determined by three integers h, k, and ℓ. The notation of (hkl) is used for a plane. This notation is called Miller indices. For a perfect single crystal, every face is parallel to a set of lattice planes. A lattice plane intersects the x, y and z axes at points a/h, b/k and c/ℓ, respectively. In other words, the Miller indices of a plane are the reciprocals of the intercepts of the plane with the crystallographic axes (Borchardt-Ott [1]). Figure 1 shows plane (211) and plane (110) in a crystallographic lattice.
A crystal form is a set of equal faces and the term habit describes the relative sizes of the faces of a crystal (Hamilton et al. [2]). The various shapes of crystals, resulting from the unequal development of their faces are called their habits (Hamilton et al. [2]). As shown in Figure 2 crystals can be grouped into 7 crystal systems (Kraus [3]). Also in Figure 2 some crystal habits are shown. Definition of every face of crystal forms have been carried out using the following equation.

\[
[hkl] [T] \begin{bmatrix} x \\ y \\ z \end{bmatrix} = d
\]

Where, [T] is the transformation matrix of the base vector of crystallographic axes and d is the distance ratio from the origin. The spacing d between adjacent (hkl) lattice planes is given for some crystal systems in the Figure 3 (wikipedia [6]).
### Crystal systems and their habits

<table>
<thead>
<tr>
<th>Crystal system</th>
<th>Spacing $d$ between adjacent (hkl) lattice planes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubic</td>
<td>$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>$\frac{1}{d^2} = \frac{4}{3} \left( \frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2}$</td>
</tr>
<tr>
<td>Rhombohedral</td>
<td>$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2) \sin^2 \alpha + 2(hk + kl + hl)(\cos^2 \alpha - \cos \alpha)}{a^2(1 - 3 \cos^2 \alpha + 2 \cos^3 \alpha)}$</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>$\frac{1}{d^2} = \frac{1}{\sin^2 \beta} \left( \frac{h^2}{a^2} + \frac{k^2 \sin^2 \beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl \cos \beta}{ac} \right)$</td>
</tr>
</tbody>
</table>

Figure 2: Crystal systems and their habits (Hamilton et al. [2])

Figure 3: Distance ratio from the origin in crystal systems (wikipedia[6])
2. Modelling of the crystals

It is convenient to have a brief survey of the method proposed in this paper in terms of an example. Consider a model of Rutile as illustrated in Figure 4. The Miller function is a mechanism whose main role is to find the intersection point of three planes. Each plane of the crystal under consideration has been represented by its Miller index in Figure 4.

The creation of a Rutile has been carried out by using the concepts of formex algebra, using the programming language Formian, as shown in Figure 5.
(*) TETRAGONAL (RUTILE) (*)

e=[4.598,4.598,2.960;90,90,90]

(*) Form 1 (*)
e1=mi1[1,1,0,0,1,0,1,0,1,0,1,-1,P,G,P,H]e
e2=mi1[1,1,0,0,1,-1,1,0,1,1,1,-1,P,H,P,D]e
e3=mi1[1,1,0,1,1,1,1,0,1,0,1,P,P,P]e
e4=mi1[1,0,1,0,-1,1,1,0,0,P,K]e
e5=mi1[1,1,0,1,0,0,1,1,0,1,1,P,P,K,P]e
e6=mi1[1,1,0,1,1,1,1,1,1,1,1,1,P,L,P]e
e7=mi1[1,1,0,1,1,1,1,0,1,1,1,P,F,F]e
e8=mi1[1,1,0,0,1,1,1,0,0,1,0,0,P,F,F]e
et1=e1#e2#e3#e4#e5#e6#e7#e8
etg1=tig(8)|et1

(*) Form 2 (*)
e9=mi0[1,1,0,1,0,1,-1,1,0,F,G,F,S]e
e10=mi0[1,1,1,1,1,1,-1,1,F,S,F,N]e
e11=mi0[1,1,1,1,1,1,-1,1,F,N,F,O]e
e12=mi0[1,1,1,1,1,1,1,F,O,F,L]e
e13=mi0[1,1,1,1,1,1,1,F,M,L,M]e
et2=e2#e#e10#e11#e12#e13
etg2=tig(7)|et2

(*) Form 3 (*)
e6=mi1[1,1,1,1,1,1,1,0,1,1,0,0,M,L,M,P]e
et3=e6#e7#e13
etg3=tig(3)|et3

(*) Form 4 (*)
e14=mi1[1,0,0,1,1,1,0,1,0,1,0,1,0,0,0,0,1,K,L,K,R]e
e15=mi1[1,0,1,1,1,0,1,0,1,0,1,0,1,0,0,0,1,K,R,K]e
et4=e4#e5#e14#e15
etg4=tig(4)|et4

clear
use vg(2),vh(14,0,1,6,9,2,8,0,1)
f1=eg1#eg4
f2=eg2#eg3
f=rosad(0,0,4,90)|f1
ff=lam(3,0)|rosad(0,0)|f2
t=f|ff
show t

Figure 5: Formulation of Rutile

The program for modelling of Rutile starts by defining a formex variable e. This formex variable represents the unit vectors of the crystallographic axes a, b and c and \( \alpha \), \( \beta \) and \( \gamma \) as angles between pairs of axes (Borchardt [1]). That is,

\[
e = [a, b, c, \alpha, \beta, \gamma]
\]

In addition, e shows the crystallographic system to which the crystal belongs. Since Rutile belongs to the tetragonal system then:

\[
a = b \neq c \quad \alpha = \beta = \gamma = 90^\circ
\]

Formex variables e1 to e8 in the Table 2 show the vertices of the plane. The details of e1 for instance are given below:

e1=mi0(h1, k1, l1, h2, k2, f2, h3, k3, f3, h1, k1, l1, P, G, P, H) e

As shown in Figure 6, a plane of Rutile (Form 1) is obtained by connecting the points (e1 to e8).
The planes of three other forms of crystal can be drawn in the same manner. Figure 7, shows the shapes of four planes of crystal which have been created.

Figure 7. Four planes of Rutile which will be used for modelling of whole crystal

Now it is time to create the whole model of the crystal by using the symmetry elements. Formian has some useful functions to do symmetry operations (Figure 8). In general a crystal can have some specific symmetry elements, which are center of inversion, axis of rotation and reflection planes.

<table>
<thead>
<tr>
<th>symmetry element</th>
<th>function name</th>
<th>imprint</th>
</tr>
</thead>
<tbody>
<tr>
<td>reflection plane</td>
<td>Lambda</td>
<td>Lam</td>
</tr>
<tr>
<td></td>
<td>reflection</td>
<td>ref</td>
</tr>
<tr>
<td>Axis of rotation</td>
<td>Rosette</td>
<td>Ros</td>
</tr>
<tr>
<td></td>
<td>vertition</td>
<td>ver</td>
</tr>
</tbody>
</table>

Figure 8: Some useful symmetry operations functions in Formian

Rutile crystallographic point group is 4/mmm, hence it has got a tetrad rotation axis and three reflection planes. Let a four-fold axis passes through e12. Rosad function makes the possibility of rotating planes 1 and 4 (f1) and planes 2 and 3 (f2) about the four-fold axis. Finally a lam function produces a mirror image of f2. f and ff together represent a whole model of Rutile. Note that just by creating of forms 1 and 2, modelling of this crystal is possible as well.
3. Generating different habits of a crystal
Miller function is able to create different habits of a crystal. For this purpose, the Miller function has been parameterised. In this regard, distance ratios of planes from the centre, determines the parameters. The result of changing the parameters is creating different habits of the crystal. Some examples of habits of Rutile are shown in Figure 9.

![Figure 9: Four habits of Rutile](image-url)
4. Conclusion
An algebraic and computational methods were used for three dimensional modelling of crystals' morphology. This method employs Formex algebra together with some crystallographic concepts. Using Formex algebra, a function called Miller function has been developed to create models of crystals. Miller function not only allows modelling of crystals but also enables creation of different habits of each crystal by changing the parameters of Miller function. Miller function has been implemented in the Formian software. According to the Formex configuration processing, Miller function allows a convenient method to designers to create their desired crystal forms.

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References