APPENDIX B

MODELING ICOSAHEDRON AND DECAHEDRON PARTICLES

B.1 Modeling Mackay Icosahedron:

(1) Build a deformed tetrahedron **T**:

A tetrahedral unit cell is defined by three basis vectors **a, b** and **c** (see figure B1). The angle between each two is 63°26'. The length of each basis vector is equal to the nearest atomic bond length *a* (e.g. 2.885 Å for Au).

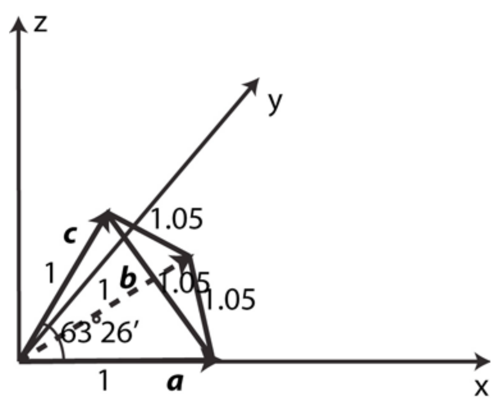

Figure B1 A deformed tetrahedron half unit cell defined by three basis vectors **a, b** and **c**. The angle between any two basis vectors is 63°26'.

Any atom position can be specified by the combination of the three basis vectors:

$$\mathbf{r}(n,m,p) = n\mathbf{a} + m\mathbf{b} + p\mathbf{c} \tag{B.1}$$

where n, m, p are three integers. Using the direction of **a** as the x-axis and plane defined by **a** and **b** as the x-y plane, one can define the Cartesian coordination, and write the atomic coordinates in terms of (n, m, p):

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} n + 0.447m + 0.449p \\ 0.894m + 0.278p \\ 0.849p \end{pmatrix} \cdot a \tag{B.2}$$

To populate atoms at the lattice sites for a given particle size N, one can specified the range of n, m, p as $0 \le p \le N$, $0 \le m \le N - p$, $0 \le n \le N - p - m$. In this way, we build a deformed tetrahedron with three edges of length N*a* and the other three edges of length 1.05 N*a*.

(2) Extend **T** to a double-tetrahedron complex

We then mirror the tetrahedron **T** about its facet defined by vector **b** and **c** (see figure B2), and form another tetrahedron **T'**.

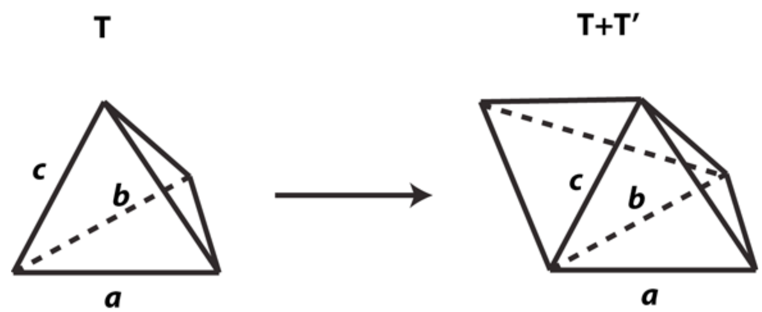

Figure B2 Mirroring the tetrahedron **T** about the **bc** plane to form a double-tetrahedron complex **T+T'**.

One way to construct **T'** is to defined another set of basis vectors for **T'**:

$$\begin{pmatrix} \mathbf{a}' \\ \mathbf{b}' \\ \mathbf{c}' \end{pmatrix} = \begin{pmatrix} \mathbf{c} \\ \mathbf{b} \\ -0.4452\mathbf{i} + 0.7244\mathbf{j} + 0.5262\mathbf{k} \end{pmatrix} \tag{B.3}$$

where **i, j, k** denotes the basis vector for the Cartesian coordination. Using B.3, one can write the coordinates in **T'** in terms of n, m, and p:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0.449n + 0.447m - 0.445p \\ 0.277n + 0.894m + 0.724p \\ 0.849n + 0.526p \end{pmatrix} \cdot a \tag{B.4}$$

Populating the lattice site in **T'** is similar to **T**.

(3) Forming the upper five-fold cap:

Now take the double-tetrahedron complex **T+T'** and rotate it for 4 times about the x axis by 72°. The rotation operation can be described by a rotation matrix:

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos 72^o & \sin 72^o \\ 0 & -\sin 72^o & \cos 72^o \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{B.5}$$

The result of this step is a five-fold cap, **C**, consisting of 10 deformed tetrahedra (see figure B3).

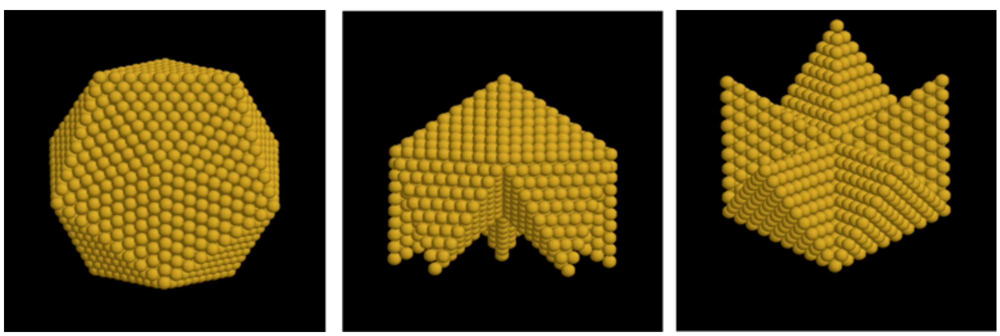

Figure B3 A five-fold cap viewed from the top (left), side (middle) and bottom (right).

(4) Generating the lower five-fold cap:

An icosahedron is made of two five-fold caps, an upper one and a lower one. The lower cap, **C'**, can be easily generated by mirroring **C** about the y-z plane:

$$\mathbf{C}' = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \mathbf{C} \tag{B.6}$$

(5) Joining **C** and **C’** to form an icosahedron:

To join the two caps just built, one needs to rotate the lower cap by 36^{o} about the x axis:

$$\mathbf{C}'' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos 36^{o} & \sin 36^{o} \\ 0 & -\sin 36^{o} & \cos 36^{o} \end{pmatrix} \mathbf{C}' \tag{B.7}$$

As a result, **C’’+C** is a complete icosahedron (see figure B4).

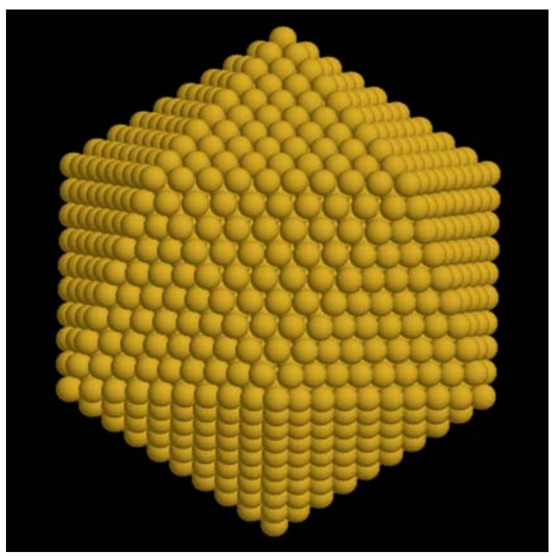

Figure B4 A completed icosahedron model.

B.2 Modeling Regular, Ino and Marks Decahedron:

Modeling decahedron is similar to icosahedron, since both are manipulation of a deformed tetrahedron, but much more simpler. For decahedron, once a deformed tetrahedron is constructed, one can form the decahedron by rotation operation. Based on different truncation schemes, regular (no truncation), Ino-type (truncations on (100) facets) and Marks-type (truncations on (100) and (111) facets) decahedra can be constructed.

(1) Building a deformed tetrahedron:

Similar to the modeling of icosahedron, we can define three basis vectors, **a, b** and **c** as illustrated in figure B5.

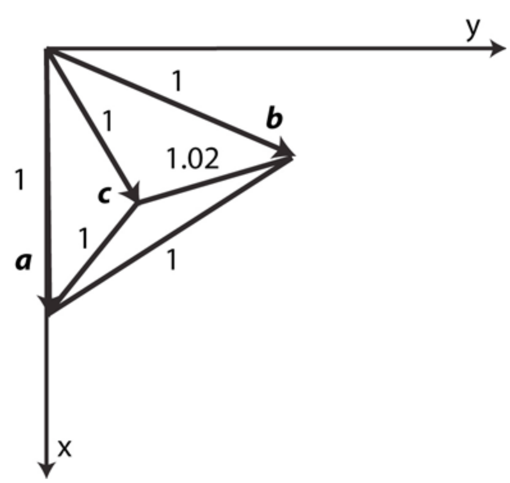

Figure B5 Definition of the three basis vectors of a deformed tetrahedron.

As shown in figure B5, the deformed tetrahedron has five edges of length a (the nearest atomic bond length) and one edge of length 1.02a. By placing the **a** vector on the x axis and the **b** vector on the x-y plane, one can define the Cartesian coordination system and write the atomic positions in terms of three integers n, m and p:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} n + 0.5(m+p) \\ 0.866m + 0.265p \\ 0.824p \end{pmatrix} \cdot a \tag{B.8}$$

By specifying different ranges for n, m and p, a deformed tetrahedron **T** with different truncation can be constructed:

i. Regular tetrahedron without any truncation (see the left panel figure B6):

$0 \le p \le N$, $0 \le m \le N - p$, $0 \le n \le N - p - m$

ii. Ino-type tetrahedron with truncation on the (100) facets (see the middle panel in figure B6): $0 \le p \le M$, $0 \le m \le M - p$, $0 \le n \le N - p - m$

Two parameters, N and M specify the size and the degree truncation.

iii. Marks-type tetrahedron with truncation on the (100) and (111) facets (see the right panel in figure B6): $0 \le p \le K$, $0 \le m \le M - p$, $0 \le n \le N - p - m$

Three parameters, N, M and K specify the size and the degree truncations.

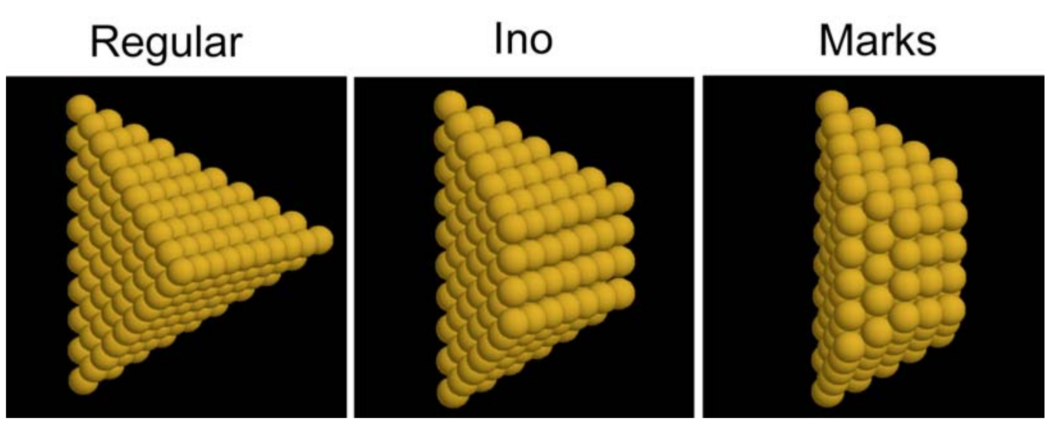

Figure B6 Constituent tetrahedron for regular (left, N=10), Ino-type (middle, N=10, M=7) and Marks-type (right, N=10, M=7 and K=5) decahedra.

(2) Forming a complete decahedron:

The complete decahedron can be constructed by rotating the constituent tetrahedron by 72^o for 4 times using the rotation matrix B.5. The resulted decahedron models are shown in figure B7.

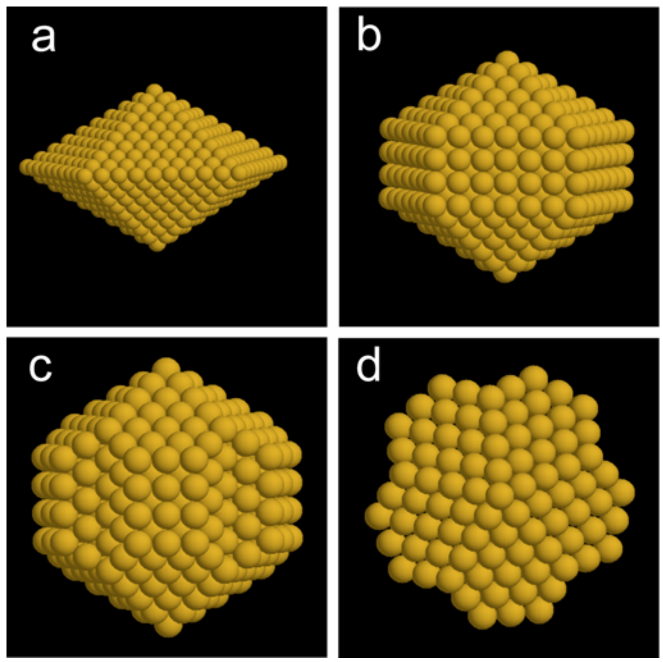

Figure B7 a. regular decahedron (N=10); b. Ino-type decahedron (N=10, M=7); c. Marks-type decahedron (N=10, M=7, K=5); d. the same Marks-type decahedron as c viewed along its five-fold axis.