Atomic Surface Generator

This program generates the atomic cordinates for slices through body-centered cubic (bcc) or face-centered cubic (fcc) solids. *a* is the lattice spacing; (*hkl*) define the Miller indices.

Parameters

$a := 4.0782 \cdot Å$	Au	Unit cell spacing (lattice spacing)
$a := 4.0853 \cdot Å$	Ag	
$h := 1$ $k := 1$ $l := 1$		Surface identifier (111), (210), etc.
$max := 10$		Cut position. ***(increase to obtain a larger surface)***
$depth := 2$		Depth of slice (number of unit cells)

Bulk Samples

$$bcc := \left| \begin{array}{l} i \leftarrow 0 \\ \text{for } z \in 0..2 \cdot max \\ \quad \text{for } y \in 0..2 \cdot max \\ \quad\quad \text{for } x \in 0..2 \cdot max \\ \quad\quad\quad \left| \begin{array}{l} M_{i,0} \leftarrow 1 \cdot \left(x + \begin{cases} 0 & \text{if } \text{even}(z) = 1 \\ 0.5 & \text{otherwise} \end{cases} \right) \\ M_{i,1} \leftarrow 1 \cdot \left(y + \begin{cases} 0 & \text{if } \text{even}(z) = 1 \\ 0.5 & \text{otherwise} \end{cases} \right) \\ M_{i,2} \leftarrow \frac{1}{2} \cdot z \\ i \leftarrow i + 1 \end{array} \right. \\ M \end{array} \right.$$

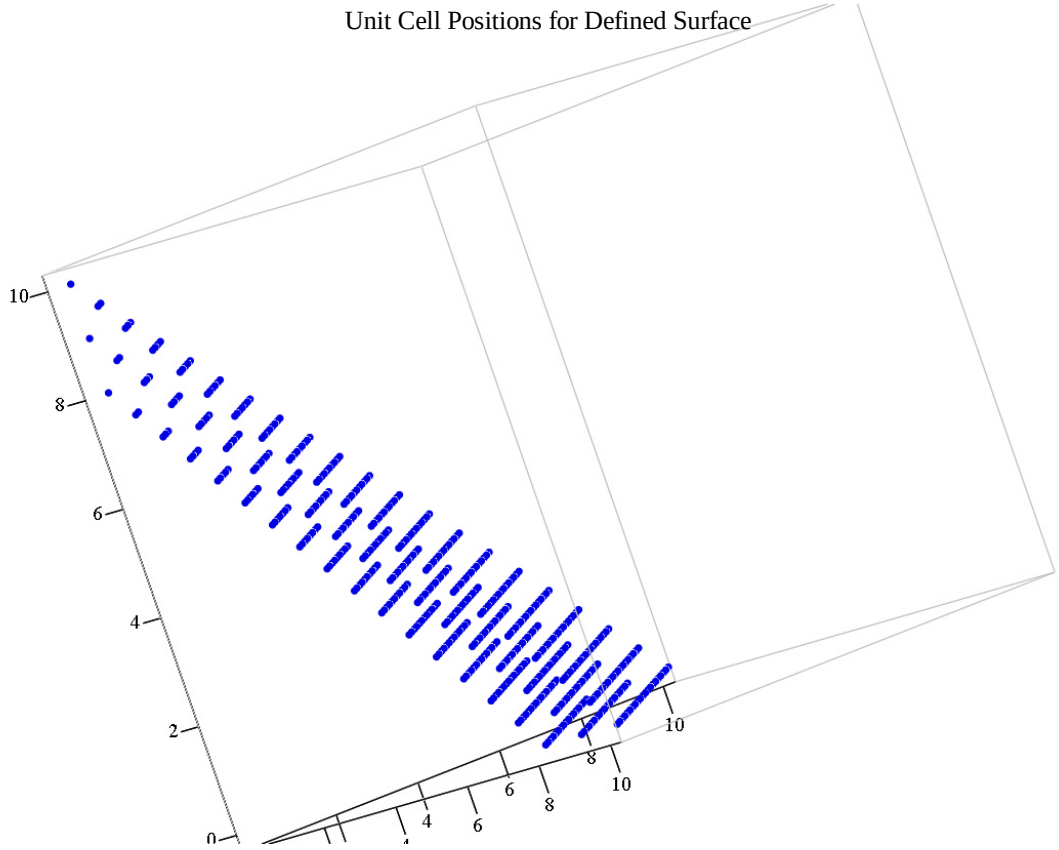
$$fcc := \left| \begin{array}{l} i \leftarrow 0 \\ \text{for } z \in 0..\frac{2 \cdot max}{2} \\ \quad \text{for } y \in 0, 0.5..2 \cdot max \\ \quad\quad \text{for } x \in 0, 0.5..2 \cdot max \\ \quad\quad\quad \left| \begin{array}{l} M_{i,0} \leftarrow x \\ M_{i,1} \leftarrow y \\ M_{i,2} \leftarrow z + \begin{cases} 0.5 & \text{if } \text{int}(x) = 0 \oplus \text{int}(y) = 0 \\ 0 & \text{otherwise} \end{cases} \\ i \leftarrow i + 1 \end{array} \right. \\ M \end{array} \right.$$

Selected Surface

bulk := fcc Selects the bulk solid.

surface :=
temp ← (0 0 0)
for j ∈ 0 .. rows(bulk) − 1
if max − h · bulk$_{j,0}$ − k · bulk$_{j,1}$ ≥ l · bulk$_{j,2}$
if max − depth − h · bulk$_{j,0}$ − k · bulk$_{j,1}$ ≤ l · bulk$_{j,2}$
temp ← stack(temp, submatrix(bulk, j, j, 0, 2))
1
1
submatrix(temp, 1, rows(temp) − 1, 0, 2)

Unit Cell Positions for Defined Surface



file := concat("(", num2str(h), num2str(k), num2str(l), ") surface.dat")

WRITEPRN(file) := surface · $\frac{a}{Å}$ Writes the atomic coordinates for the above surface to file.

file = "(111) surface.dat"

