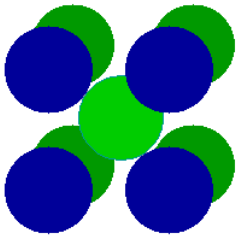
1.5: Surface Structures- bcc metals

A number of important metals (e.g. Fe, W, Mo) have the bcc structure. As a result of the low packing density of the bulk structure, the surfaces also tend to be of a rather open nature with surface atoms often exhibiting rather low coordination numbers.

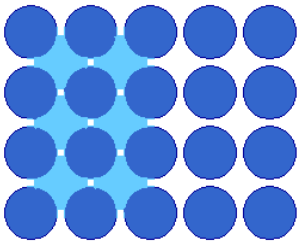
I. The bcc (100) surface

The (100) surface is obtained by cutting the metal parallel to the front surface of the bcc cubic unit cell - this exposes a relatively open surface with an atomic arrangement of 4-fold symmetry.



bcc unit cell (100) face

The diagram below shows a plan view of this (100) surface - the atoms of the second layer (shown on left) are clearly visible, although probably inaccessible to any gas phase molecules.

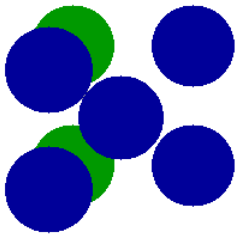


bcc (100) surface plane, e.g. Fe(100)

- What is the coordination number of the surface layer atoms on the bcc(100) surface?
- Is the coordination of the second layer atoms the same as that of bulk atoms ?

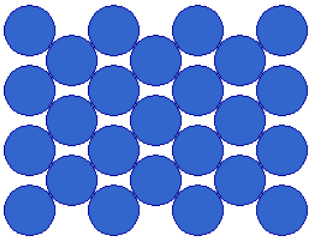
II. The bcc (110) surface

The (110) surface is obtained by cutting the metal in a manner that intersects the x and y axes but creates a surface parallel to the z-axis - this exposes a surface which has a higher atom density than the (100) surface.



bcc unit cell (110) face

The following diagram shows a plan view of the (110) surface - the atoms in the surface layer strictly form an array of rectangular symmetry, but the surface layer coordination of an individual atom is quite close to hexagonal.

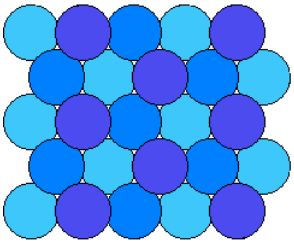


bcc(110) surface plane, e.g. Fe(110)

- What is the coordination number of the surface layer atoms on the bcc(110) surface?

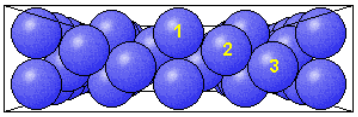
III. The bcc (111) surface

The (111) surface of bcc metals is similar to the (111) face of fcc metals only in that it exhibits a surface atomic arrangement exhibiting 3-fold symmetry - in other respects it is very different.



Top View: bcc(111) surface plane e.g. Fe(111)

In particular it is a very much more open surface with atoms in both the second and third layers clearly visible when the surface is viewed from above. This open structure is also clearly evident when the surface is viewed in cross-section as shown in the diagram below in which atoms of the various layers have been annotated.



Side View: bcc(111) surface plane, e.g. Fe(111)