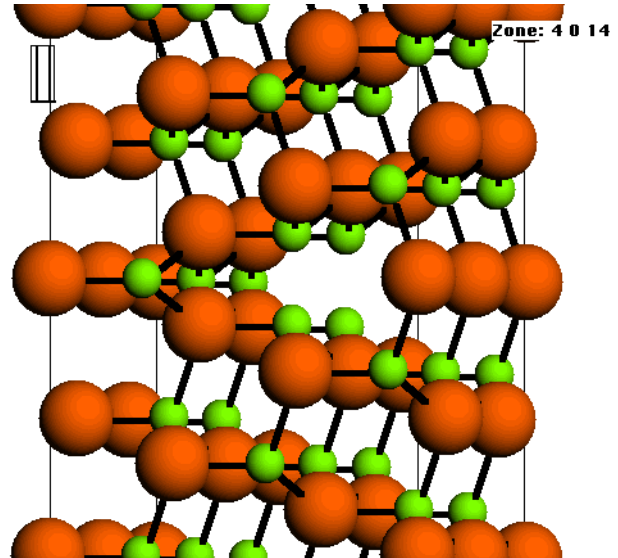


# CrystalKit

**CrystalKit** is a new product from the creator of MacTempas. It is a program that dramatically decreases the time involved in building crystalline defects of various kinds, from point defects to grainboundaries and precipitates. The program starts from single crystal data, which can be entered within the program or read in from structure files used with the MacTempas program. Any final structure generated by CrystalKit can be saved in a MacTempas file for immediate simulation of diffraction patterns and High Resolution TEM images. The program accepts up to 2 different crystalstructures for creating interface structures. A geometric grainboundary involving several thousand atoms can be generated in a matter of minutes by specifying the orientation relation between the grains, the interface plane and the zone-axis. CrystalKit allows the user to freely rotate the crystal to show different views. There



are tools to identify planes, measure angles and distances between atoms, visually move atoms, delete atoms and add new atoms. There is even a tool to create an arbitrary path interface. Sections of atoms can be removed as a whole and pasted into the structure. One crystalline structure can become a precipitate in another structure. In the end when the user has arranged the structure to his/her satisfaction, a unit cell can be marked with the "Define Unit Cell Tool". This unit cell can then be written out as a MacTempas structure file ready for further work.

CrystalKit allows the display of up to four different atomic bonds between atoms and the color and atomic radius are easily changed.

