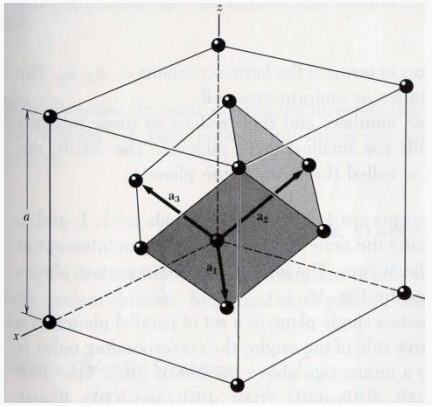
Chapter 3 Hands-on Excises

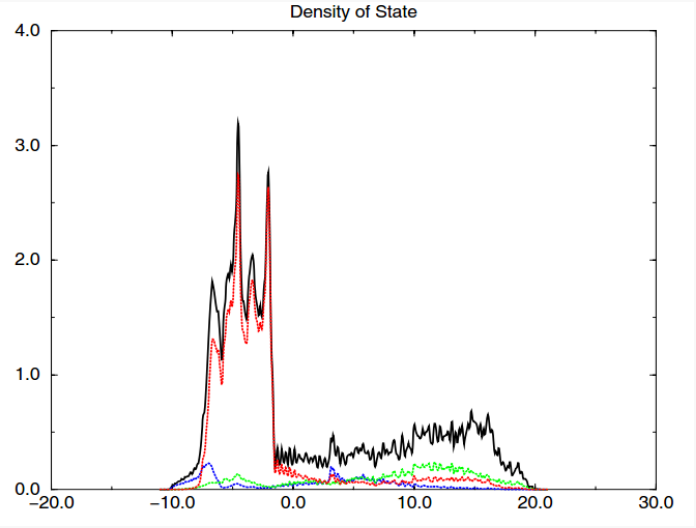
3.1 Using VASP program to calculate the electronic structure of bulk nonmagnetic materials



1. fcc Au

a) Self-consistent electronic structure calculation:
The lattice constant is fixed, a = 4.08 Å .
Perform the SCF calculations and then take a look at the OUTCAR.

b) Create another directory called, e.g., DOS. With the CHGCAR fixed (ICHARG = 11, LCHARG = .FALSE.), calculate the total and s, p, d orbital decomposed densities of states; Plot the densities of states using “xmgrace”.



c) Create another directory called, e.g., “BAND”. With the CHGCAR fixed (ICHARG = 11, LCHARG = .FALSE.), calculate the energy bands along the high symmetry lines in the fcc Brillouin zone. Plot the energy bands using “xmgrace”.

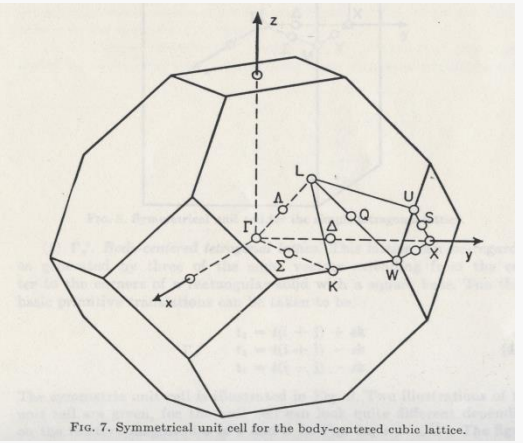
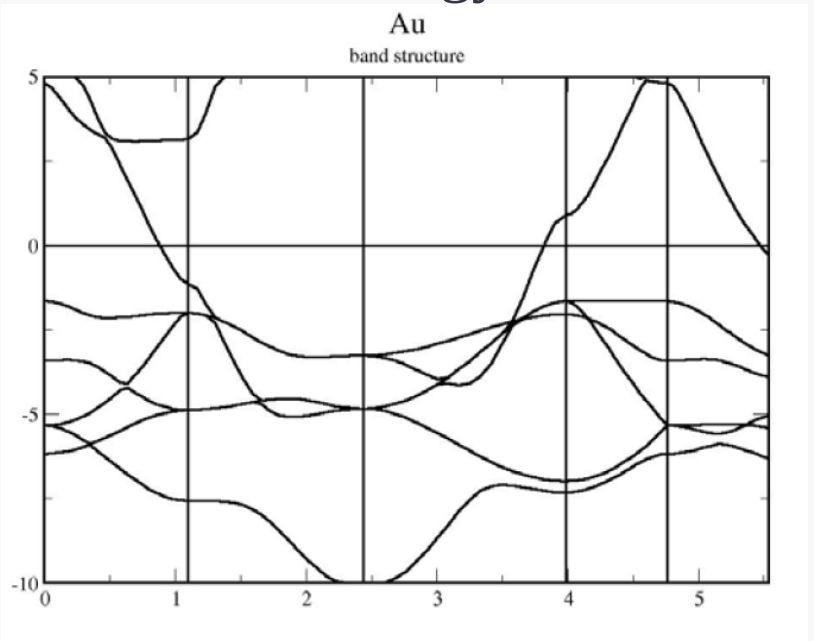
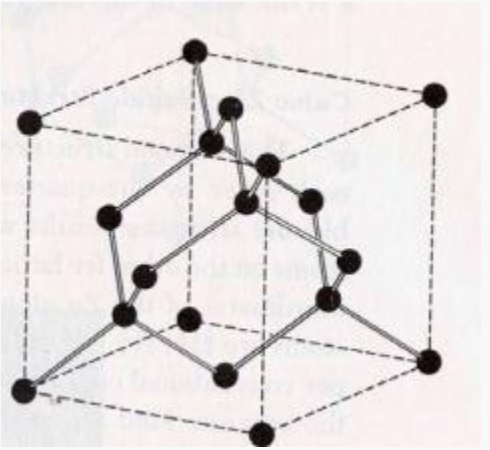


FIG. 7. Symmetrical unit cell for the body-centered cubic lattice.



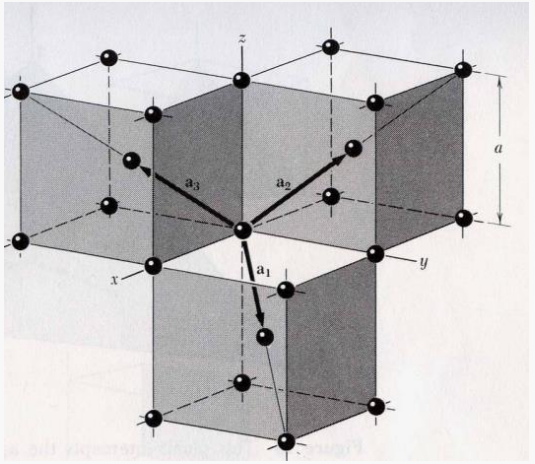
2. Homework:

Perform the same calculations for Si in diamond structure.



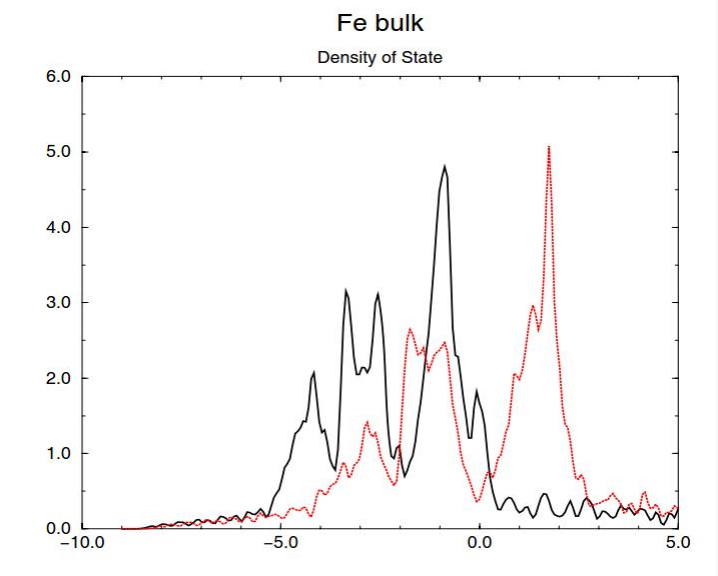
3.2 Using VASP program to calculate the electronic structure of bulk ferromagnetic materials

1. bcc Fe



a) Self-consistent spin-polarized electronic structure calculation: The lattice constant is fixed, a = 2.87 Å . Perform the SCF calculations and then take a look at the OUTCAR.

b) Create another directory called, e.g., DOS. With the CHGCAR fixed (ICHARG = 11, LCHARG = .FALSE.), calculate the total and s, p, d orbital decomposed densities of states; Plot the densities of states using “xmgrace”.



c) Create another directory called, e.g., “BAND”. With the CHGCAR fixed (ICHARG = 11, LCHARG = .FALSE.), calculate the energy bands along the high symmetry lines in the fcc Brillouin zone. Plot the energy bands using “xmgrace”.

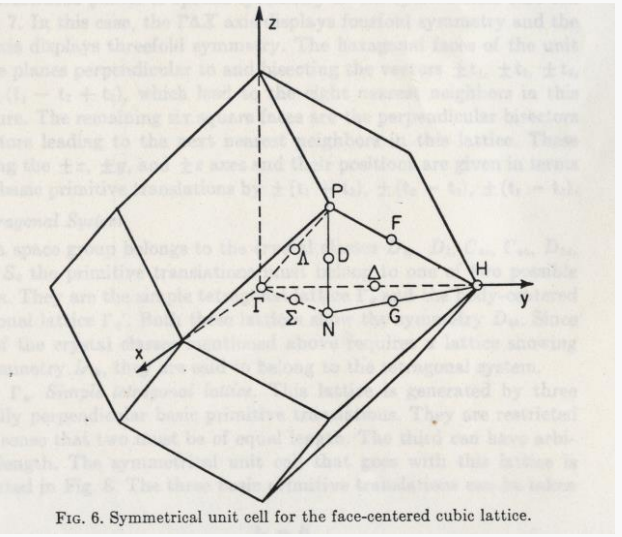
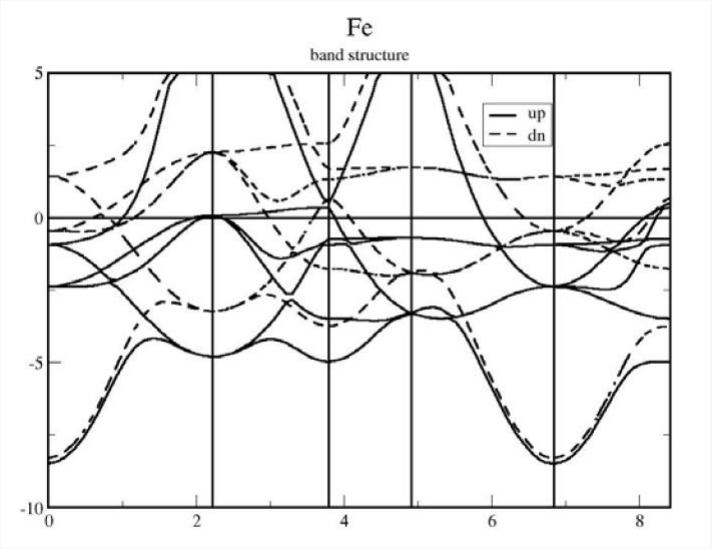


FIG. 6. Symmetrical unit cell for the face-centered cubic lattice.



2. Homework:
   Perform the same calculations for fcc Ni.