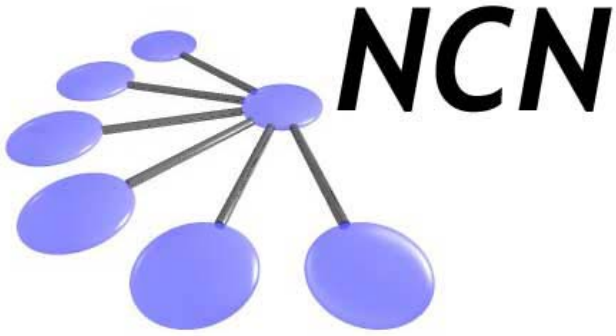
Tutorial 4B – Device Simulation: Metals



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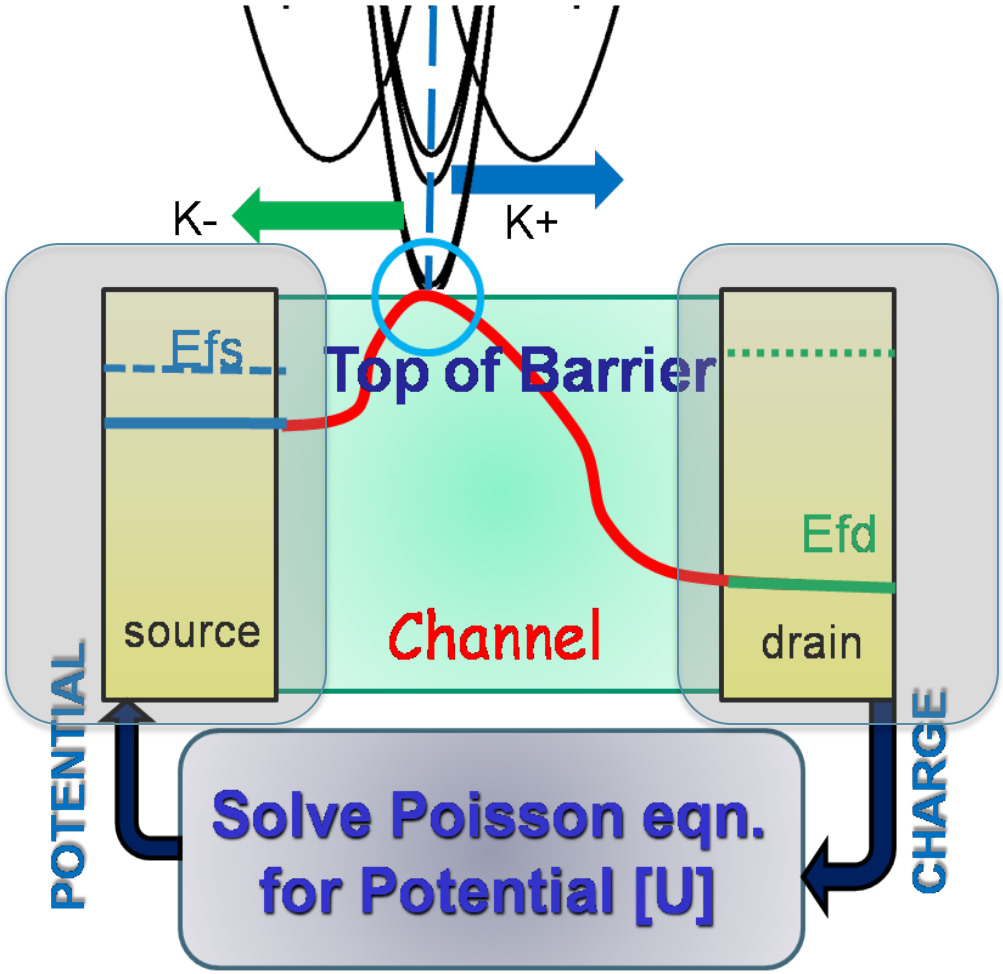
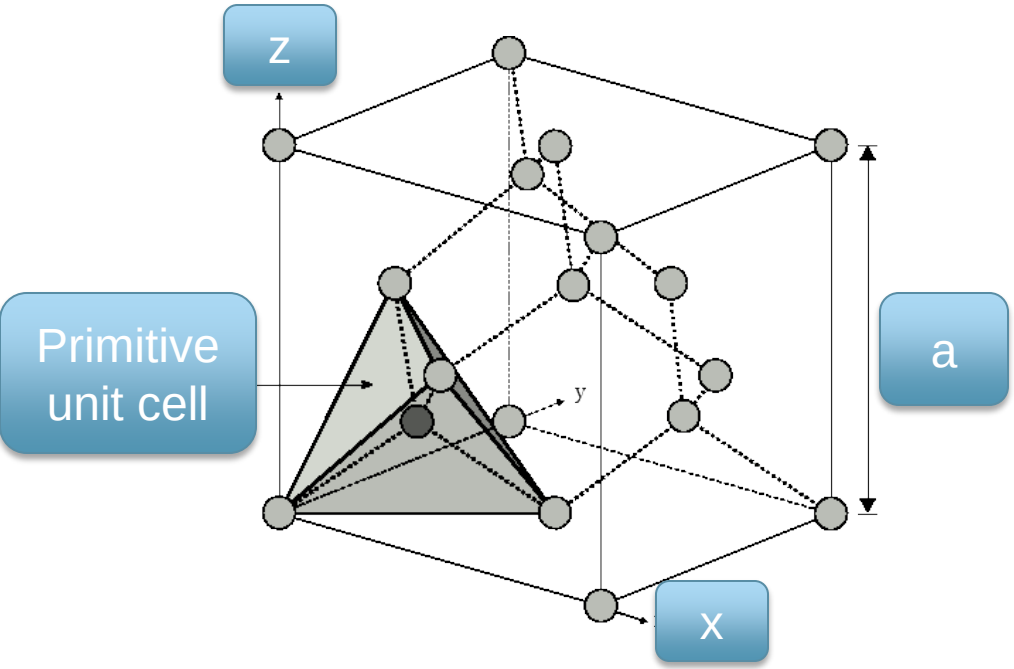
Metals in device modeling – existing paradigm



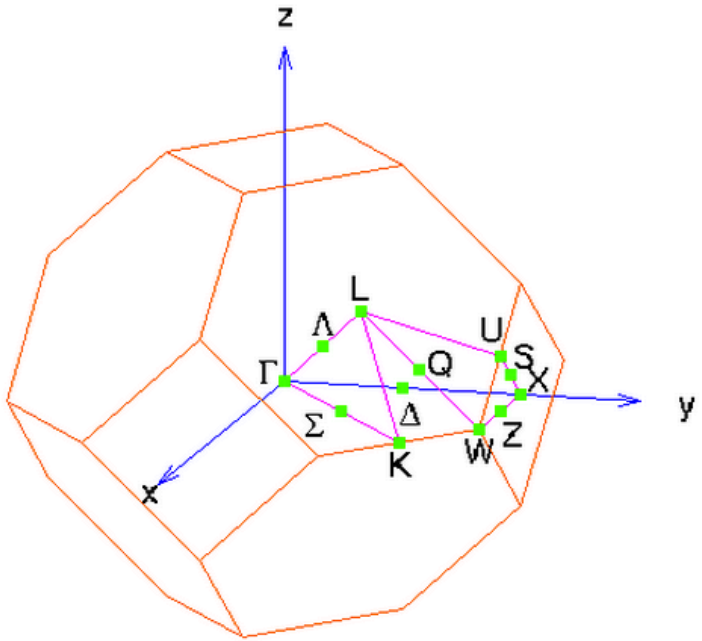
- Metal – used to set Fermi Level in device
- Either abstracted out or treated using effective mass approximation
- As devices continue to scale, the metal needs to be treated atomistically
- We are trying to bring metals into the device modeling paradigm uasing NEMO5

Image from https://engineering.purdue.edu/gekcogrp/research-group/AbhijeetPaul/project3.php with kind permission of Abhijeet Paul

FCC Metal Unit Cell and Brillouin Zone



- Single atom in Primitive Unit Cell at origin - say (0,0,0)
- Primitive Lattice Vectors –
  - (0.5 0.5 0)*a/2
  - (0.5 0 0.5)*a/2
  - (0 0.5 0.5)*a/2



- Reciprocal Lattice is BCC
- We would like to plot band structure along following directions in the 1st Brillouin Zone (Gamma -> X -> W -> L -> Gamma -> K)

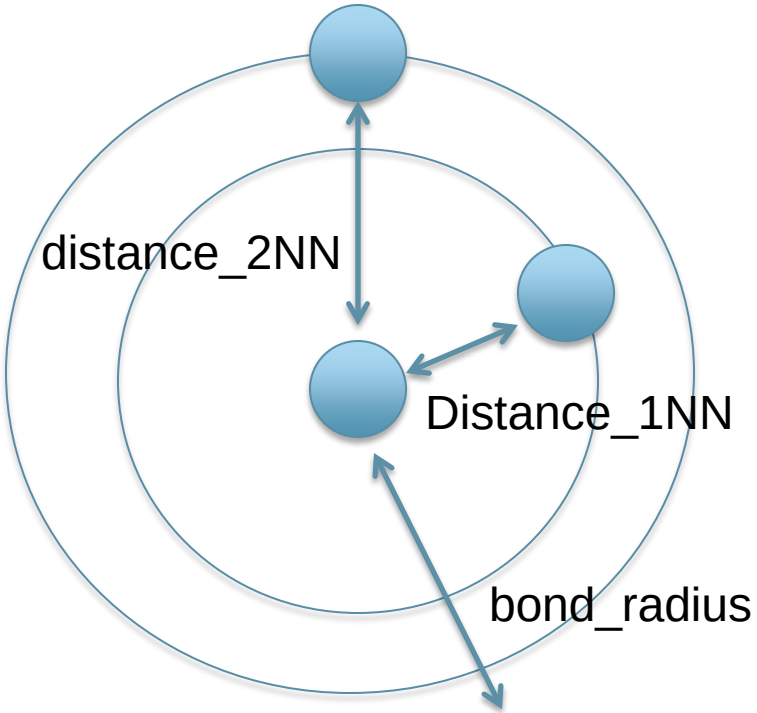
Images from http://www.iue.tuwien.ac.at/phd/ungersboeck/img682.png and http://cst-www.nrl.navy.mil/bind/kpts/fcc/index.html

Setting up input deck for bulk Cu – structure options

Materials Section

```
Material
    {
        name = Cu
        tag = substrate
        crystal_structure = fcc
        regions = (1)
        neighbor_coupling = 2NN
        bond_radius = 0.37
        distance_1NN = 0.26
        distance_2NN = 0.37
        //which TB parameter set?
        Bands:TB:sp3d5sstar:param_set = NRL_2NN_Orthogonal

    }
```



Domain options

```
Domain
    {
        name = structure1
        type = pseudomorphic
        base_material = substrate
        dimension = (1,1,1)
        periodic = (true, true, true)
        crystal_direction1 = (1,1,0)
        crystal_direction2 = (0,1,1)
        crystal_direction3 = (1,0,1)
        space_orientation_dir1 =  (1,1,0)
        space_orientation_dir2 =  (0,1,1)
        passivate=false
        regions = (1)
        geometry_description = simple_shapes
    }
```

Geometry

```
Geometry
        {
                Region
                {
                        shape         = cuboid
                        region_number = 1
                        priority      = 1
                        min           = (-5,-5,-5) // in nm
                        max           = ( 5, 5, 5)
                        tag = substrate
                }
        }
```

Solvers

```
solver
        {
                name          = Cu
                type          = Schroedinger
                domain        =  structure1
                active_regions = (1)
                job_list      = (calculate_band_structure)
                output        = (energies, k-points)
                tb_basis = sp3d5sstar
                use_monomials = false
                Matlaboutput = false
                chem_pot      = 0.0
                shift         = 0.0
                // full band structure Gamma-X-W-L-Gamma-K
                k_space_basis   = reciprocal
                k_points =
[(0,0,0),(0.5,0,0.5),(0.5,0.25,0.75),(0.5,0.5,0.5),(0,0,0),(0.375,0.375,0.75)]
                number_of_nodes = (100,100,100,100,100)
        }
```

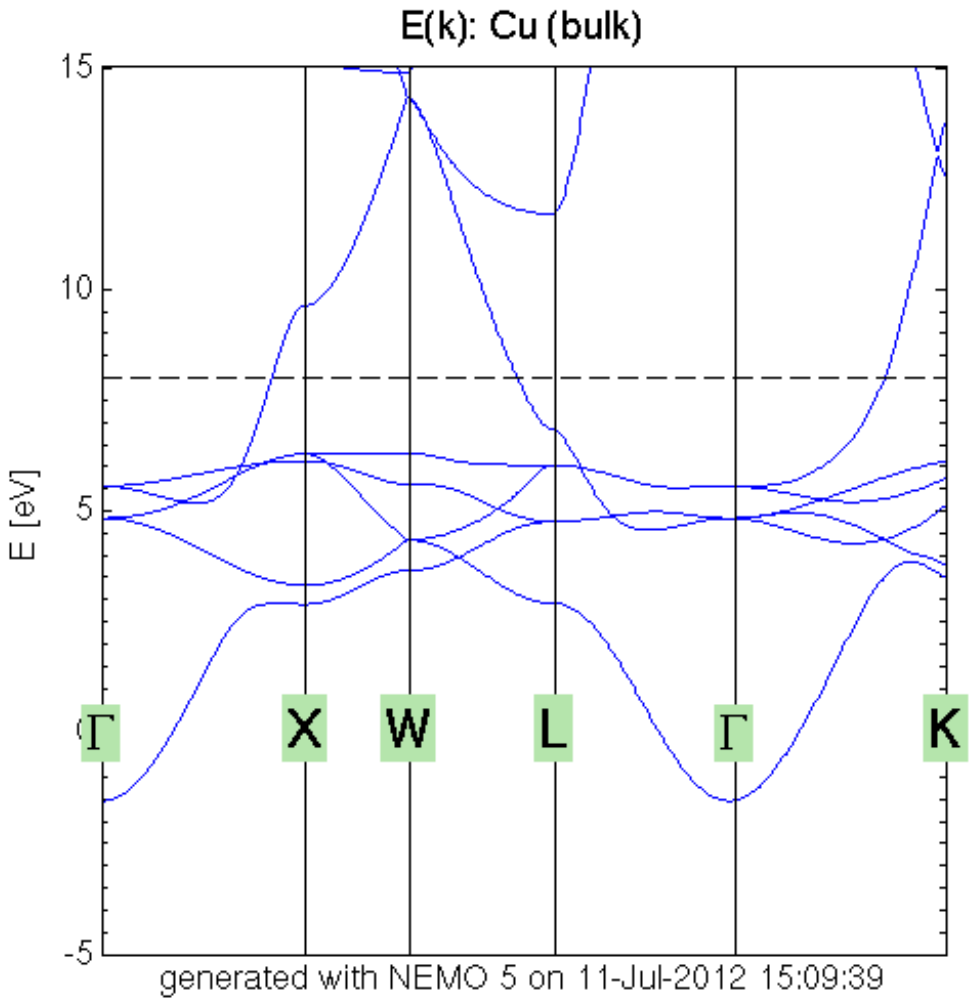
Global section

```
Global
{
        solve    = (Cu)
        database = ../../../../materials/all.mat
}
```

Exercise 3 – metal bulk band structure

- Log in to your workspace account
- Retrieve the file ***Cu_bulk.in*** from folder ***/apps/share64/nemo/examples/current/public_examples/bulk_Cu*** :
- ***Cu_bulk.in*** will execute a NEMO5 job to calculate the dispersion relationship for the bulk Cu unit cell that you just set up
- Create a symbolic link to the database file using the following command:
  - ***ln -s /apps/share64/nemo/examples/current/materials/all.mat***
- Execute it on nanoHUB using the submit command
  - ***submit -v coates -i ./all.mat nemo-r7962 Cu_bulk.in***
- Retrieve the matlab file plot_bands.m from folder ***/apps/share64/nemo/examples/current/public_examples/bulk_Cu*** and copy into the directory you just executed in.
- You should see files of the type ***Cu_*.dat.*** Make sure the file '***Cu_energies.dat'*** exists.
- Load matlab in your workspace account using '***use matlab-7.12***' followed by '***matlab***'. cd into the local directory where you executed nemo.
- Execute plot_bands.m with the following arguments passed to it –
  - ***plot_bands('Cu',-5,15,8.0223);***

You should get the following result



Try this example with other metals too

- name = ‘Ag’ / ‘Au’ / ‘Al’ – in the materials section.
- The lattice parameters are 0.409/ 0.408/ 0.405 nanometers respectively.
- The distance_1NN are <lattice_parameter>/sqrt(2).
- distance_2NN = lattice_parameter.
- Everything else remains the same.
- Try it out!
- *You can modify this input deck to plot bulk band structure for other semiconductors having FCC unit cells too.*
- *Remove the neighbor_coupling, bond_radius, distance_1NN, distance_2NN options, change the material name and the Bands:TB:sp3d5sstar:param_set options. The rest remains the same.*

- Metal-Semiconductor TB parameters
- Transport through M-S junctions.
- Metal alloy TB parameters
- And lots more…!!