

```

clc
clear

Type = 'FCC';
element = 'Ni';
a0 = 3.524;
mass = 63.5460;

atom1 = [0.0 * a0, 0.0 * a0, 0.0 * a0];
atom2 = [0.5 * a0, 0.5 * a0, 0.0 * a0];
atom3 = [0.5 * a0, 0.0 * a0, 0.5 * a0];
atom4 = [0.0 * a0, 0.5 * a0, 0.5 * a0];

ux = [1.0 * a0, 0.0, 0.0];
uy = [0.0, 1.0 * a0, 0.0];
uz = [0.0, 0.0, 1.0 * a0];

id = 0;

for i = -10:10
    for j = -10:10
        for k = -10:10
            vector = ux * i + uy * j + uz * k;
            id = id + 1;
            crystal(id, 1:3) = atom1 + vector;
            id = id + 1;
            crystal(id, 1:3) = atom2 + vector;
            id = id + 1;
            crystal(id, 1:3) = atom3 + vector;
            id = id + 1;
            crystal(id, 1:3) = atom4 + vector;
        end
    end
end

rand_list = randperm(id);
Ni_atoms_indices = rand_list(1:id / 2);
Al_atoms_indices = rand_list((id / 2 + 1):id);

Ni_id = 1;
Al_id = 1;
for i = 1:id
    if find(Ni_atoms_indices == i)
        Ni_crystal(Ni_id, 1:3) = crystal(i, 1:3);
        Ni_id = Ni_id + 1;
    else
        Al_crystal(Al_id, 1:3) = crystal(i, 1:3);
        Al_id = Al_id + 1;
    end
end

plot3(Ni_crystal(:, 1), Ni_crystal(:, 2), Ni_crystal(:, 3), 'o', 'MarkerFaceColor','g', 'MarkerSize', 10);
axis square;
hold on;
plot3(Al_crystal(:, 1), Al_crystal(:, 2), Al_crystal(:, 3), 'o', 'MarkerFaceColor','b', 'MarkerSize', 10);
axis square;
hold off;

```

