```
% Open source on 开源于
% https://github.com/Techy-Wu/MATLAB-learning/tree/8f7d3a6a3edda5ad190737fc7fd204305d90a95e/FCC%E6%9B%BF%E6%8D%A2

% 初始化工作区
clc
clear

% 基础变量
Type = 'FCC';
element = 'Ni';
a0 = 3.524;
mass = 58.693;

% 定义晶胞原子
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];

% 定义基矢量
ux = [1.0 * a0, 0.0, 0.0];
uy = [0.0, 1.0 * a0, 0.0];
uz = [0.0, 0.0, 1.0 * a0];

% 循环生成
id = 0;
for i = 0:10
    for j = 0:10
        for k = 0:10
            % 得到位移矢量
            vector = ux * i + uy * j + uz * k;
            % 由晶胞原子出发沿位移矢量添加原子
            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

% 裁切生成的晶格以符合仅10个胞
crystal = lattice_slicer(crystal, [0.0, 0.0, 0.0], [a0*10, a0*10, a0*10]);
% 更新晶格矩阵长度
id = length(crystal);

% 生成序号的随机全排列数列
rand_list = randperm(id);
% 按比例分配随机数号段
Ni_atoms_indices = rand_list(1:ceil(id / 2));
Al_atoms_indices = rand_list((ceil(id / 2) + 1):id);
fprintf('Total amount of Ni atoms: %d\n', length(Ni_atoms_indices));
fprintf('Total amount of Al atoms: %d\n', length(Al_atoms_indices));

% 遍历查找并拾取对应原子
Ni_id = 1;
Al_id = 1;
for i = 1:id
    if find(Ni_atoms_indices == i)
        % 序号属于Ni号段
        Ni_crystal(Ni_id, 1:3) = crystal(i, 1:3);
        Ni_id = Ni_id + 1;
    else
        % 序号属于Al号段
        Al_crystal(Al_id, 1:3) = crystal(i, 1:3);
        Al_id = Al_id + 1;
    end
end

% MATLAB作图
% 作图并保存句柄
Ni_plot = plot3(Ni_crystal(:, 1), Ni_crystal(:, 2), Ni_crystal(:, 3), 'o', 'MarkerFaceColor','g', 'MarkerSize', 10);
% 方正化坐标
axis square;
% 锁定作图
```

```
hold on;
Al_plot = plot3(Al_crystal(:, 1), Al_crystal(:, 2), Al_crystal(:, 3), 'o', 'MarkerFaceColor','b', 'MarkerSize', 10);
axis square;
% 取消锁定
hold off;
% 添加图例，并定位在图右侧(East side)
legend([Ni_plot, Al_plot], 'Ni Atom', 'Al Atom', 'Location', 'eastoutside');

% 输出pdb和txt
% 打开文件并保存句柄
pdb_file_ID = fopen('FCC-NiAl lattice.pdb', 'w');
txt_file_ID = fopen('FCC-NiAl lattice.txt', 'w');
% 定义文件格式
rasmol_format_spec = '%-6s%-5d %-4s%-1s%-3s  %-4d%-1s   %-8.3f%-8.3f%-8.3f\n';
table_format_spec = '%-5s\t%-8.3f\t%-8.3f\t%-8.3f\n';
% 循环输出各原子坐标信息
num = 0;
for id = 1:length(Ni_crystal)
    num = num + 1;
    fprintf(pdb_file_ID, rasmol_format_spec, 'ATOM', num, element, ' ', ' ', 1, ' ', Ni_crystal(id, 1), Ni_crystal(id, 2), Ni_crystal(id, 3));
    fprintf(txt_file_ID, table_format_spec, '1', Ni_crystal(id, 1), Ni_crystal(id, 2), Ni_crystal(id, 3));
end
num = 0;
for id = 1:length(Al_crystal)
    num = num + 1;
    fprintf(pdb_file_ID, rasmol_format_spec, 'ATOM', num, 'Al', ' ', ' ', 1, ' ', Al_crystal(id, 1), Al_crystal(id, 2), Al_crystal(id, 3));
    fprintf(txt_file_ID, table_format_spec, '2', Al_crystal(id, 1), Al_crystal(id, 2), Al_crystal(id, 3));
end
% 关闭文件
fclose(pdb_file_ID);
fclose(txt_file_ID);

% 晶格裁切函数
function output_lattice = lattice_slicer(input_lattice, min_limit, max_limit)
    id = 1;
    for i = 1:length(input_lattice)
        if sum(input_lattice(i, 1:3) >= min_limit) == 3 && sum(input_lattice(i, 1:3) <= max_limit) == 3
            output_lattice(id, 1:3) = input_lattice(i, 1:3);
            id = id + 1;
        end
    end
end
```

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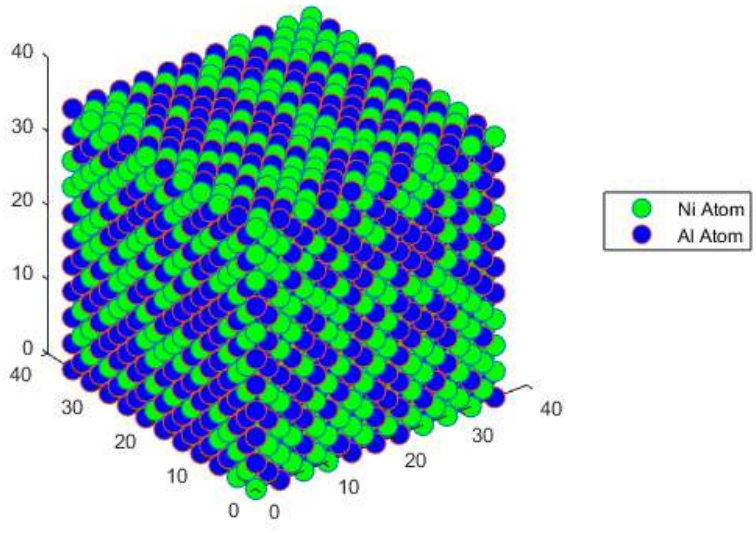
Total amount of Ni atoms: 2316
Total amount of Al atoms: 2315
```



Published with MATLAB® R2023b