# Aluminium

**Group 3A and 3B**

## 1 Input set-up

Aluminium (Al) is a silvery-white, soft, non-magnetic and ductile metal in the boron group. Aluminium has a FCC crystal structure with an experimental lattice parameter of 4.05 Å.

- generate an input file for an SCF computation: you should decide which pseudopotential you will use (norm-conserving, ultrasoft, PAW), the approximation for the exchange-correlation potential (LDA, PBE, PBE-sol) and the smearing model (fermi-dirac, gaussian, mp or mv).
- visualize your crystal structure with the software XCRYSDEN. This will help you understand if you are going to simulate the correct system or not with the input file you have written!

## 2 Convergence tests

- Set a sufficiently high grid sampling in k-space (e.g. $6 \times 6 \times 6$) and vary the value of $E_{\text{cut}}$. Be careful that you must also change the value of $E_{\text{rho}}$ if you are using US or PAW pseudopotentials! Then plot the total energy per atom as a function of $E_{\text{cut}}$. We say that the energy is converged when its variations are $\leq 1$ mRy. What is your converged $E_{\text{cut}}$?
- Now set $E_{\text{cut}}$ to the value which assures convergence as found at precedent point. Vary both the k-point grid and the smearing value. Plot the total energy per atom as a function of the number of k-points. What is your converged k-point grid? What is your converged value of the smearing?
- Perform an automatic cell+ion relaxation: what is the new lattice parameter? what are the new ions' positions? Compare the theoretical lattice parameters with their experimental counterparts. What is the error? What is the cause?

## 3 Electronic structure

Starting from either the theoretical relaxed structure or the experimental structure, both with the converged parameters:

- Perform a band computation and extract the electronic dispersion relation. By fitting band minima or maxima with a parabola you can extract the effective masses of carriers. Moreover, by fitting bands near the Fermi level with a line, you can estimate the Fermi velocity;
- Perform a non-self consistent computation with increasing value of the k-point grid and extract the electron density of states until convergence is reached. Plot the converged result and discuss if the system can be considered free-electron like. Moreover extract the value of the density of states at the Fermi level.
- Finally plot the shape of the Fermi surface with Xcrysden and try to compare it with the electronic band structure. Can you say what is the nature (electronic or holonic) of the Fermi sheets?

## 4 Vibrational properties

- Perform a convergence test for phonons at $q = \Gamma$: change the k-grid in the SCF cycle and for each case perform a phonon computation until convergence of phonon frequencies is reached.
- With the converged k-grid, perform a phonon computation on a coarse grid of q-points, for example you can start with $2 \times 2 \times 2$. Extract the phonon dispersion relation and the phonon density of states. From this you can fit acoustic modes with lines, whose slope will give you the sound velocity. Moreover, from the density of states you can get an estimate of both the Debye and Einstein temperature.
- Now increase the grid of q-points and see if phonon dispersion relation and density of states change.

## 5 Superconductivity

- Make an SCF calculation using a dense grid of k-points: for example you can use the converged grid od the NSCF you found precedently. The dense grid must contain all k and k+q grid points used in the subsequent electron-phonon calculation and must be dense enough to produce accurate electron-phonon coefficients. Insert the option la2F=.true. in the &SYSTEM namelist to instructs the code to save data into a *.a2Fsave file, subsequently read during the electron-phonon calculation.

- Make an SCF calculation using a grid of k-points that is suitable for good self-consistency and phonon calculation.

- Make the phonon and electron-phonon calculation for the grid of q-points. The input variable electron phonon=interpolated tells the ph.x code to do a linear interpolation of the electron-phonon matrix element using a double grid technique and the variable fildvscf tells the code where the derivative of the potential should be stored.

- Bring the force constant and electron-phonon coefficient to real space using a Fourier transformation with the q2r.x program. Add also here the option la2F=.true.

- Calculate $\gamma_{q\nu}$ on selected lines using the program matdyn.x. For this you need to have the input variables dos=.false. and la2F=.true.

- Calculate the electron-phonon coupling strength $\lambda_{q\nu}$ on selected hight symmetry lines and the Eliashberg spectral function $\alpha_2 F(\omega)$ using the program matdyn.x. For this you need to have the input variables dos=.true. and la2F=.true. Check convergence of quantities and plot the Eliashberg spectral function

- Finally compute the value of the total electron-phonon coupling constant and the superconducting ctitical temperature using the program lambda.x. What is the converged value of $\lambda$ and $T_c$? Which value of the pseudopotential did you use?