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Computational Condensed Matter Physics - Makeup exam

1: Preliminary steps:

- Here, I choose to work with the binary metallic alloys NiSi.

2. Electronic properties of hypothetical AB compounds in the B2 structure, ground-state structure:

2.1Initial Structure Setup and Convergence of the Relevant Input Parameters:

2.1.1

- We have 2 inequivalent Wyckoff positions. Both of them have the 1 multiplicity. They are fixed positions. Their point group is m-3m.

- We would have the Body centered cubic lattice structure, and the space group is 229.

- The space group is built up from point group + translation (depended on the underlying Bravais lattice), included rotations, reflections, and inversions, lattice translations, glide planes, and screw axes

2.1.2-4

- Initial set up, binary metallic alloys NiSi, cubic lattice constant 6 a.u
- Because we don't know our system are metal or insulator, we use the Methfessel–Paxton smearing method with a fixed smearing value of 0.04 Ry to perform our simulations
- We will start the convergence test with a total energy accuracy of 20 meV for one atom. I have two atoms, so in total my total energy is 40 meV

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   restart_mode = 'from_scratch'
   prefix = '${atoms}'
   tstress = .true.
   tprnfor = .true.
   pseudo_dir = './PSEUDO'
   outdir = './tmp'
&end
&SYSTEM
   ibrav = 1
   nat = 2
   ntyp = 2
   celldm(1) = 6
   ecutwfc = $ECUT !90

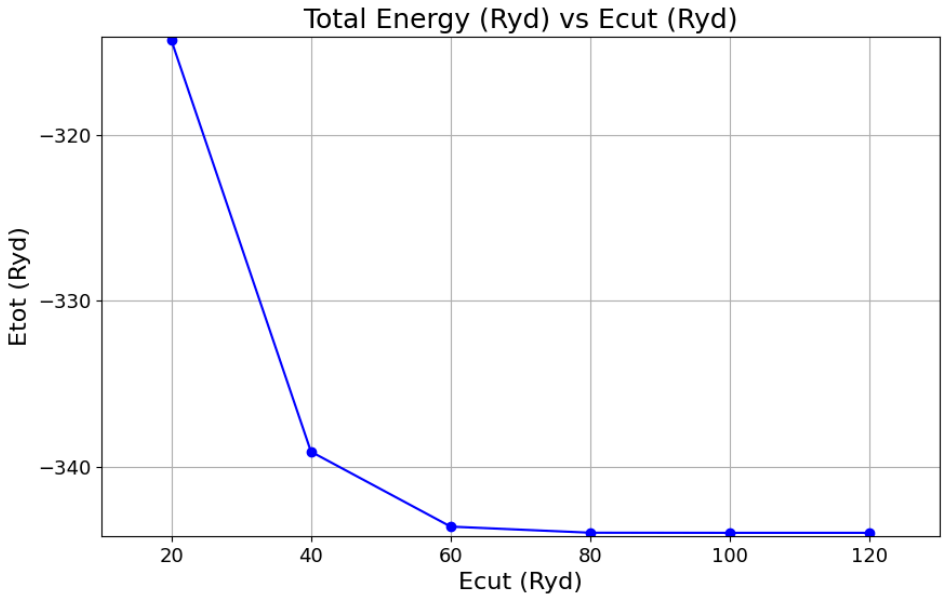
&end
&ELECTRONS
   conv_thr =  1e-06
&end
ATOMIC_SPECIES
   Si  28.0855    Si.upf
   Ni   58.6934    Ni.upf
ATOMIC_POSITIONS crystal
   Si     0.0     0.0     0.0
   Ni     0.5     0.5     0.5
K_POINTS automatic
${ks}  ${ks}  ${ks}    0  0  0
```

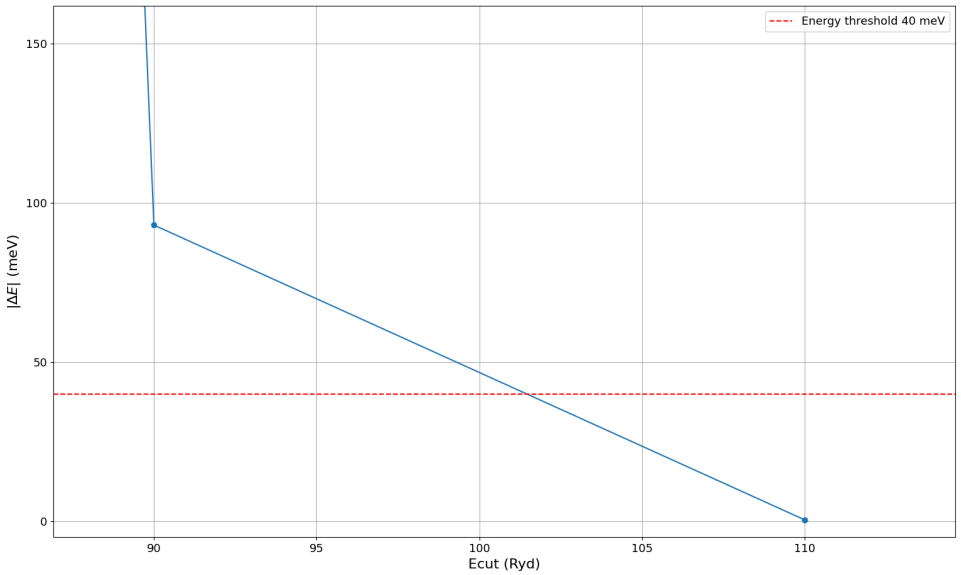
We create the template file of template.SiNi.in inside the template folder and we would use the convergence_test_on_Ecut.sh and convergence_test_on_kmesh.sh bash files to do the convergence test respectively to find the energy cut the limit of our plane wave, and the k-mesh - the resolution of our grid inside the brillouin zone.

Atomic mass

Si	Ni
28.0855 u	58.6934

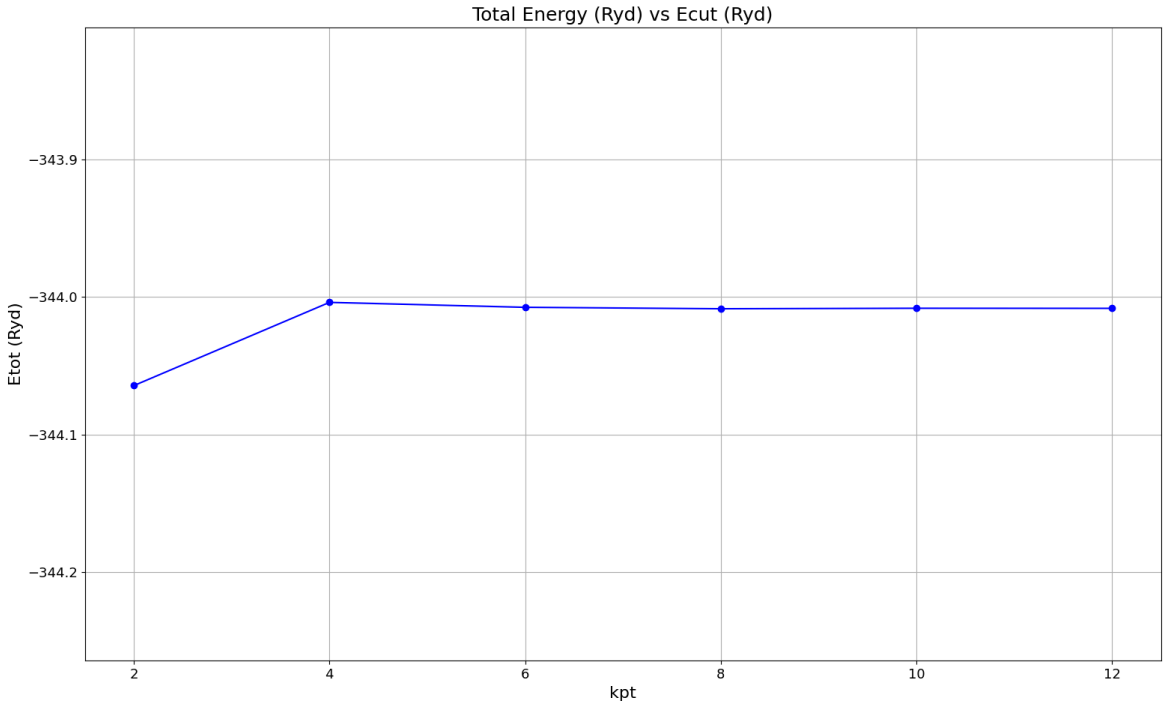
First, I do the convergence test with Ecut, the absolute relative change of the energy is below under 40meV at Ecut = 110 Ryd. I chose this as the cut-off of my plane wave.

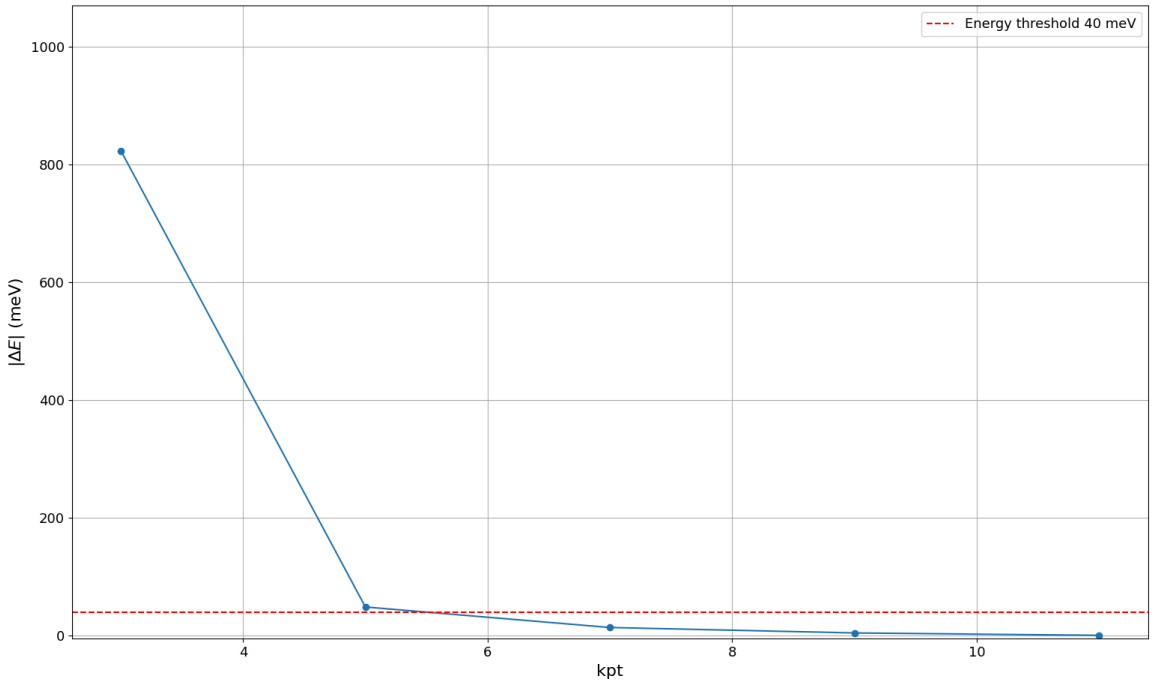




Second, I use this Ecut and vary the k-point to find the convergence value. As you can see in the image below, the total energy equilibrium near the number of k-points are

7.





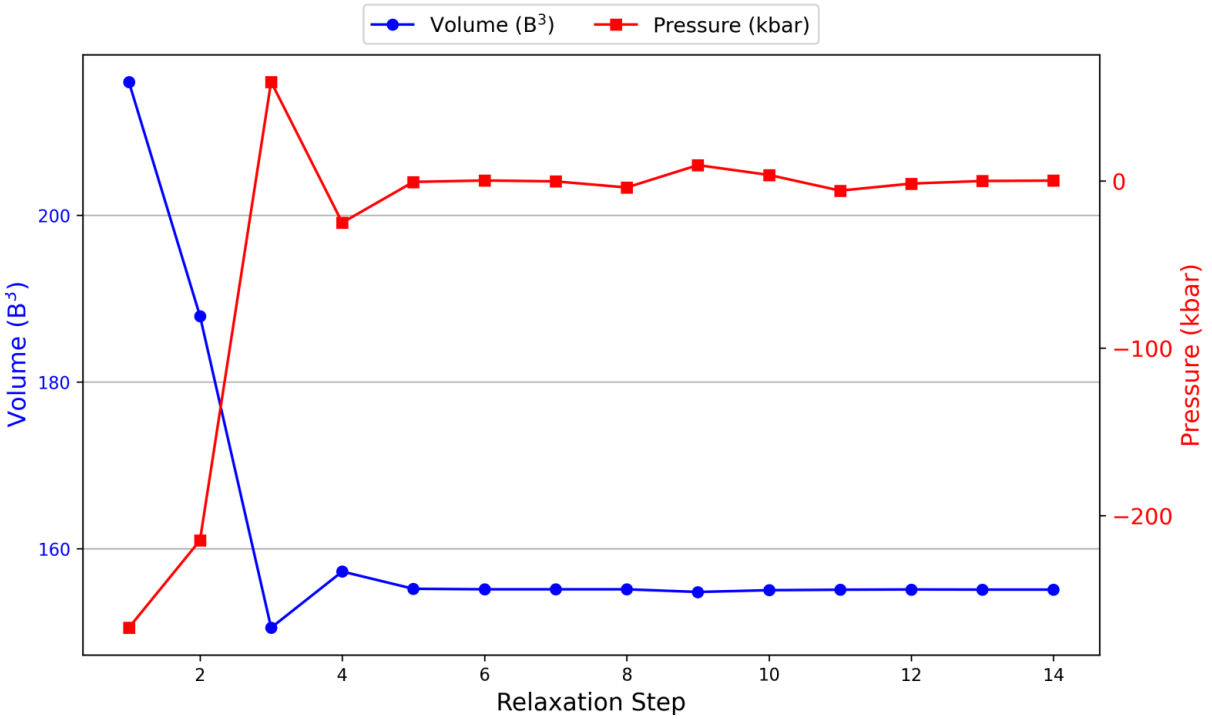
Summary, after the convergence test, we have Ecut=110 Ryd and k-point = 7.

2.2 Electronic properties of the ground-state structure

- Structure relaxation means our structure is not in the equilibrium structure, we are in the global and minima of potential energy surface, which is defined as a function of the atom positions. In a minimum structure, we will have zero force and stress. In structure optimization, we optimize the atom positions and lattice parameters to minimize the stress and force, using algorithms

such as finite difference. To boost the process further, Quantum Expresso utilises the Hellman-Feynman theorem to derivatives of the total energy respectively to atom positions and cell deformation respectively.

- Our setup pressure is -266.93 kbar, we don't have any force acting on the atoms. Because our pressure is negative, I expect my volume will shrink after the relaxation process. As I expect, after the relaxation process, the volume shink to 155.10261(a.u.)^3, with the lattice constant 5.373 a.u. After 14 steps, 7 steps for the first relaxation and another 7 steps for second relaxation.



3. Strain

3.1

- You can find my setup file of SiNi with in-plane strain $\epsilon = -0.1$, at the 3.2 folder, SiNi.scf.in

3.2+3.3

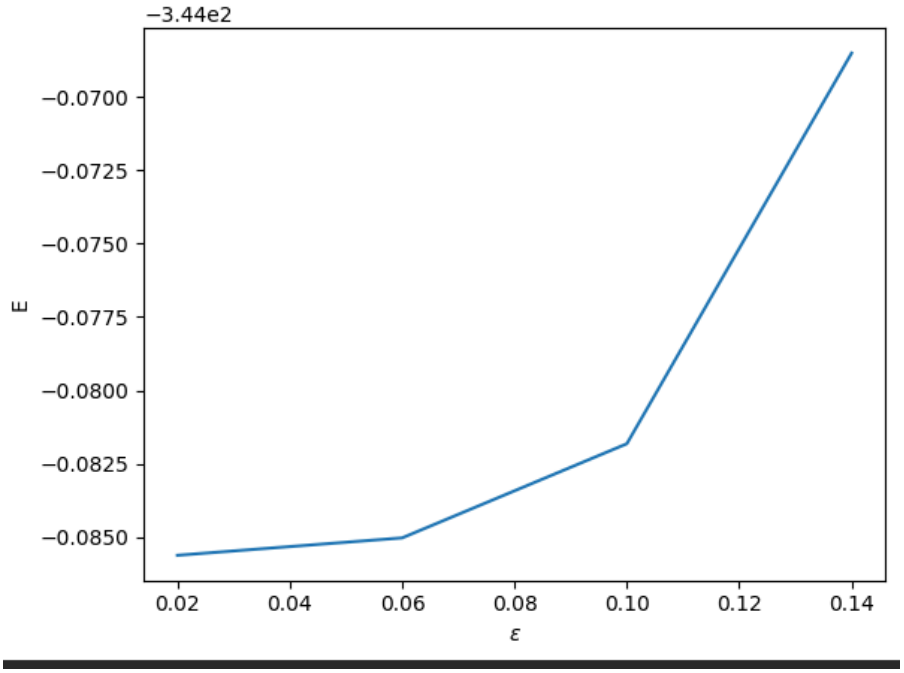
After the self-consistent calculation, I got

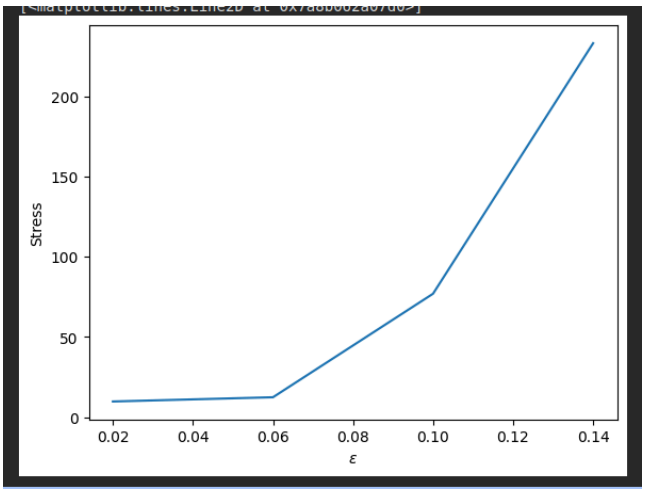
Volume	Total energy	Stress tensor (kbar)
125.6422 (a.u.)^3	-344.03767054 Ry	• $\sigma_{xx} = 561.63$ • $\sigma_{yy} = 561.63$ • $\sigma_{zz} = 607.56$

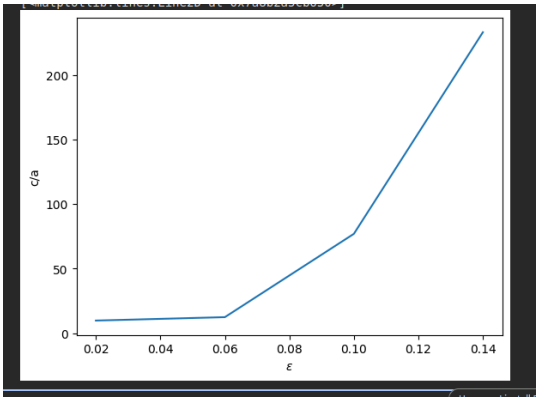
All of the diagonal stress tensors are positive, because we make our volume smaller by introducing the in-plane strain, our stress needs to be positive, because it is

similar to how we put some force on our crystal. If we let the unit cell relax in the z direction, it would elongate or expand. The volume increases to 149.58076 B^3, c/a increases to 1.19032779.
3.4

in-plane strain	volume	c/a ratio	total energy	σ_{xx}	σ_{yy}	σ_{zz}
-0.02	154.3173 (a.u.)^3	1.0357 1001	-344.08562 075 Ry	9. 71	9.71	-0.52
-0.06	153.2813 (a.u.)^3	1.1181 74118	-344.08502 773 Ry	12 .3 5	12.35	2.83
-0.1	149.5808 (a.u.)^3	1.1903 27794	-344.08182 011 Ry	76 .8 8	76.88	0
-0.14	143.3686 (a.u.)^3	1.2494 9089	-344.06851 287 Ry	23 3. 01	233.01	1.11







Here, we produce three plots of the energy vs. strain, in-plane stress vs. strain, and c/a ratio vs. strain.

For the $(E,\ \epsilon)$, my energy minimum is at 0, we don't have the supersoft for this model. When we apply the strain the c/a increases quadratically.

- My plot does agree with the equation 1-2, my stress is proportional to the derivative of the energy respectively to the strain.