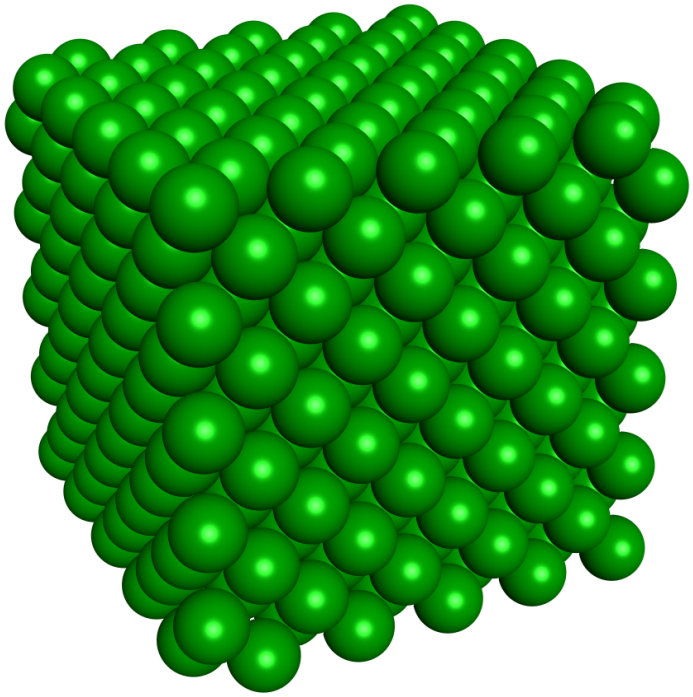
Phonon calculation (PHONON)

1. Calculation setup

The following setup is used.

- Method : PHONON
- Potential : EAM (embedded atom method)
- System : Ni crystal (supercell: primitive cell x 5)
- k-points : 50 points for dispersion curve in [100] direction
  20x20x20 points for the density of states

The crystal structure (face-centered-cubic) is shown below.

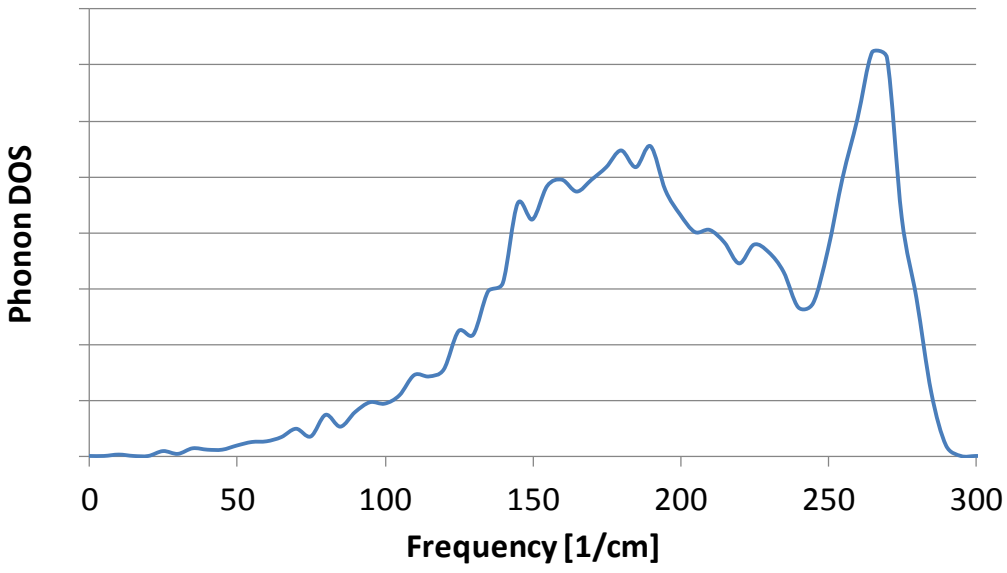


2. Results

The phonon density of states (DOS) is printed in “phonon_dos.out”.

```
========================
 [cm**-1]     phonon dos
------------------------
   0.00     0.00000000
   5.00     0.00000000
  10.00     0.25000000
  15.00     0.00000000
  20.00     0.00000000
  25.00     0.87500000
  30.00     0.37500000
  35.00     1.37500000
  40.00     1.12500000
  45.00     1.12500000
  50.00     1.87500000
  55.00     2.50000000
  60.00     2.62500000
  65.00     3.37500000
  70.00     4.87500000
  75.00     3.50000000
  80.00     7.37500000
  85.00     5.25000000
  90.00     7.87500000
     ...omitted...
```

The following figure shows the plot of phonon DOS.



The phonon dispersion along the reciprocal vector designated by the keyword <kdisp_phonon> is printed in “phonon_kdisp.out”.

kx [/bohr]	ky [/bohr]	kz [/bohr]	num	[cm**-1]
0.000000	0.000000	0.000000	1	-0.00
0.000000	0.000000	0.000000	2	290.56
0.000000	0.000000	0.000000	3	290.56
0.000000	0.000000	0.000000	4	290.56
0.000000	0.000000	0.000000	5	-0.00
0.000000	0.000000	0.000000	6	-0.00
0.000000	0.000000	0.000000	7	212.71
0.000000	0.000000	0.000000	8	212.71
0.000000	0.000000	0.000000	9	212.71
0.000000	0.000000	0.000000	10	212.71
0.000000	0.000000	0.000000	11	212.71
0.000000	0.000000	0.000000	12	212.71
0.009450	0.000000	0.000000	1	4.99
0.009450	0.000000	0.000000	2	290.52
...omitted...				

The phonon dispersion along [100] direction is shown below.