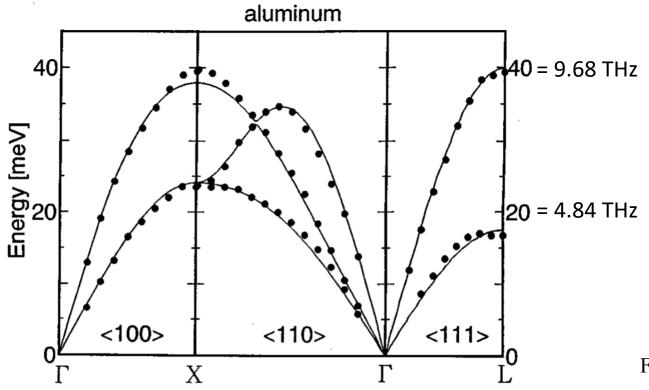
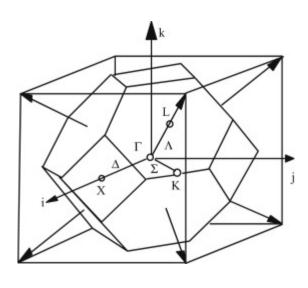
Aluminum Phonon Dispersion





Face-centered Cubic Brillouin Zone

https://en.wikipedia.org/wiki/Brillouin_zone

Aluminum:

$$k_{TF} = 2 \text{ Å}^{-1}$$
 $k_{F} = 0.175 \text{ Å}^{-1}$
 $k_{BZ} = 0.78 \text{ Å}^{-1}$
 $\frac{\omega_{i,p}}{2\pi} = 28.6 \text{ THz}$

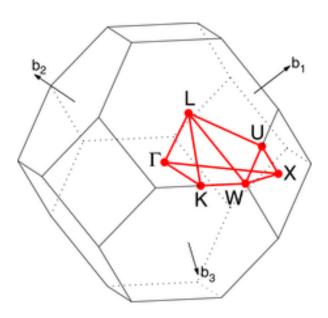
FIG. 1. The solid lines denote the calculated bulk phonon dispersions of Al by a force constant model. In spite of the small number of the fitting parameters used in this calculation (two stretching and two tangential SFC's up to 2NN bonds), the overall agreement between the calculated dispersion curves and the measured ones by inelastic neutron scattering (filled circles) is reasonably good.

Wave Vector

 $1 \text{ meV} = 0.242 \text{ THz} = 8.066 \text{ cm}^{-1}$

https://doi.org/10.1103/PhysRevB.55.10064

R. Stedman and G. Nilsson, "Dispersion relations for phonons in aluminum at 80 and 300 K", <u>Phys. Rev. 145</u>, 492 (1966).



FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X
[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]