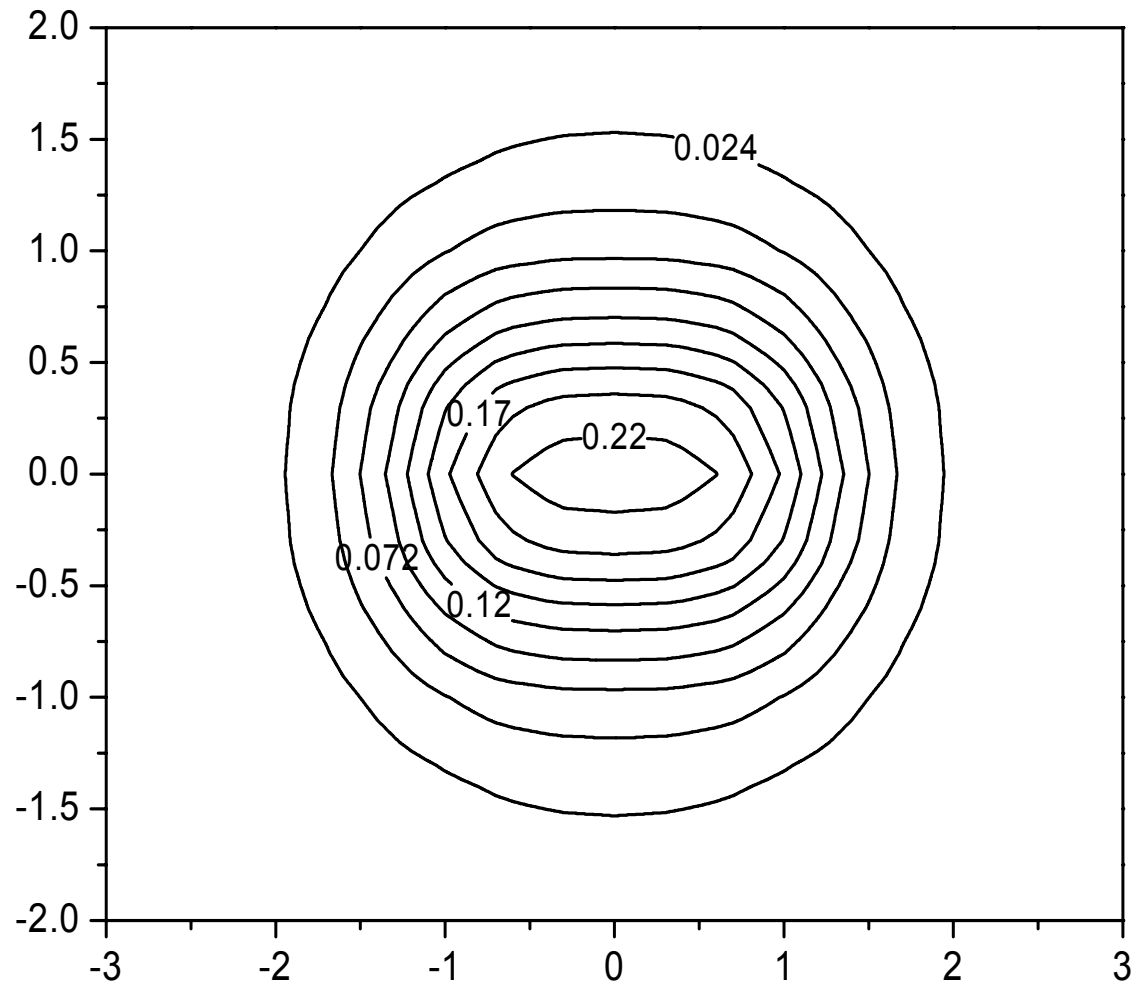


H₂ density from
t14o_DEN
using program cut3d
-3<x<3, -2<y<2, z=0
(Mathematica plot)



H₂ density from $\tau_{14\text{o_DEN}}$ using program cut3d (Origin plot)



SPACE GROUPS

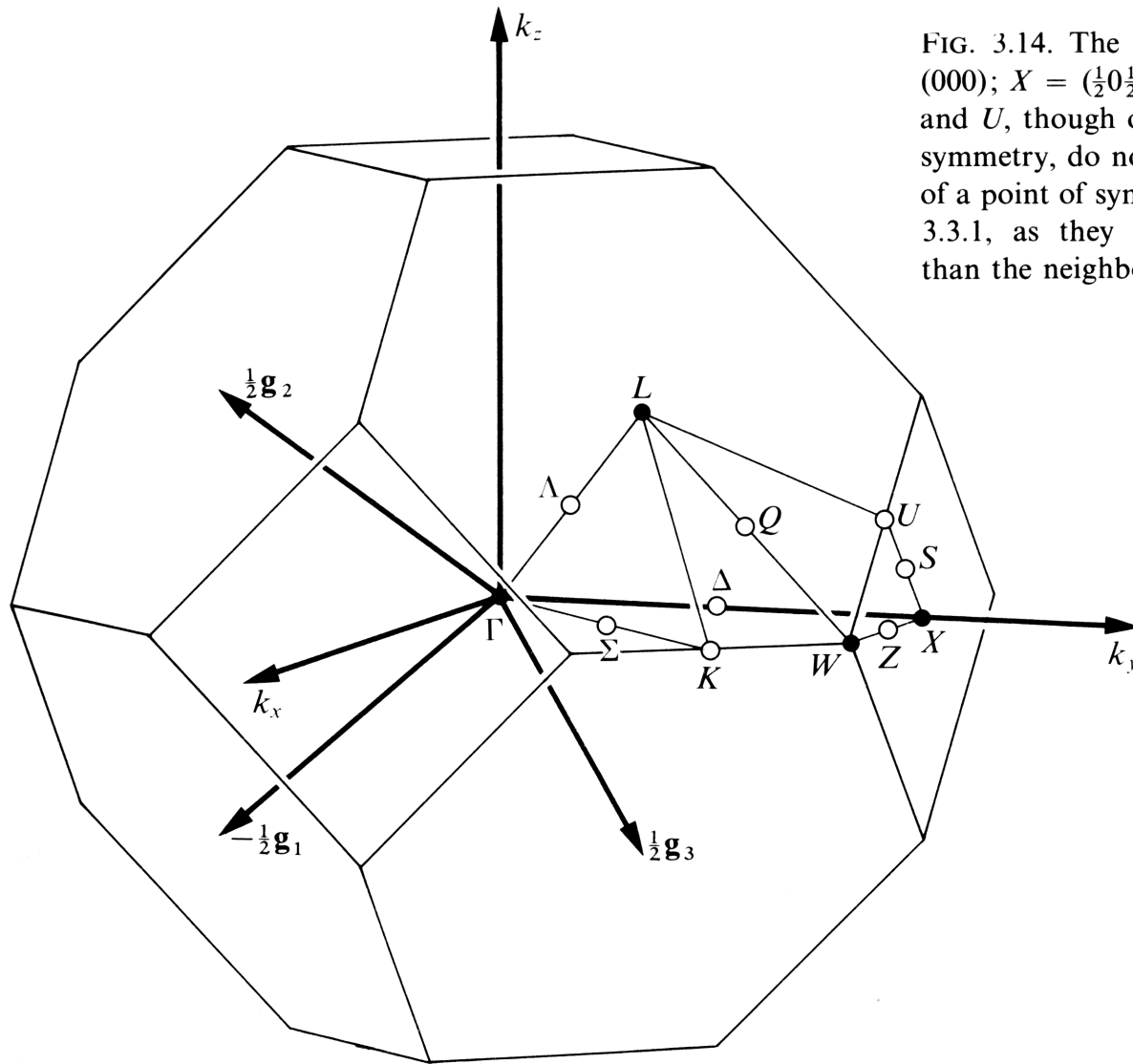
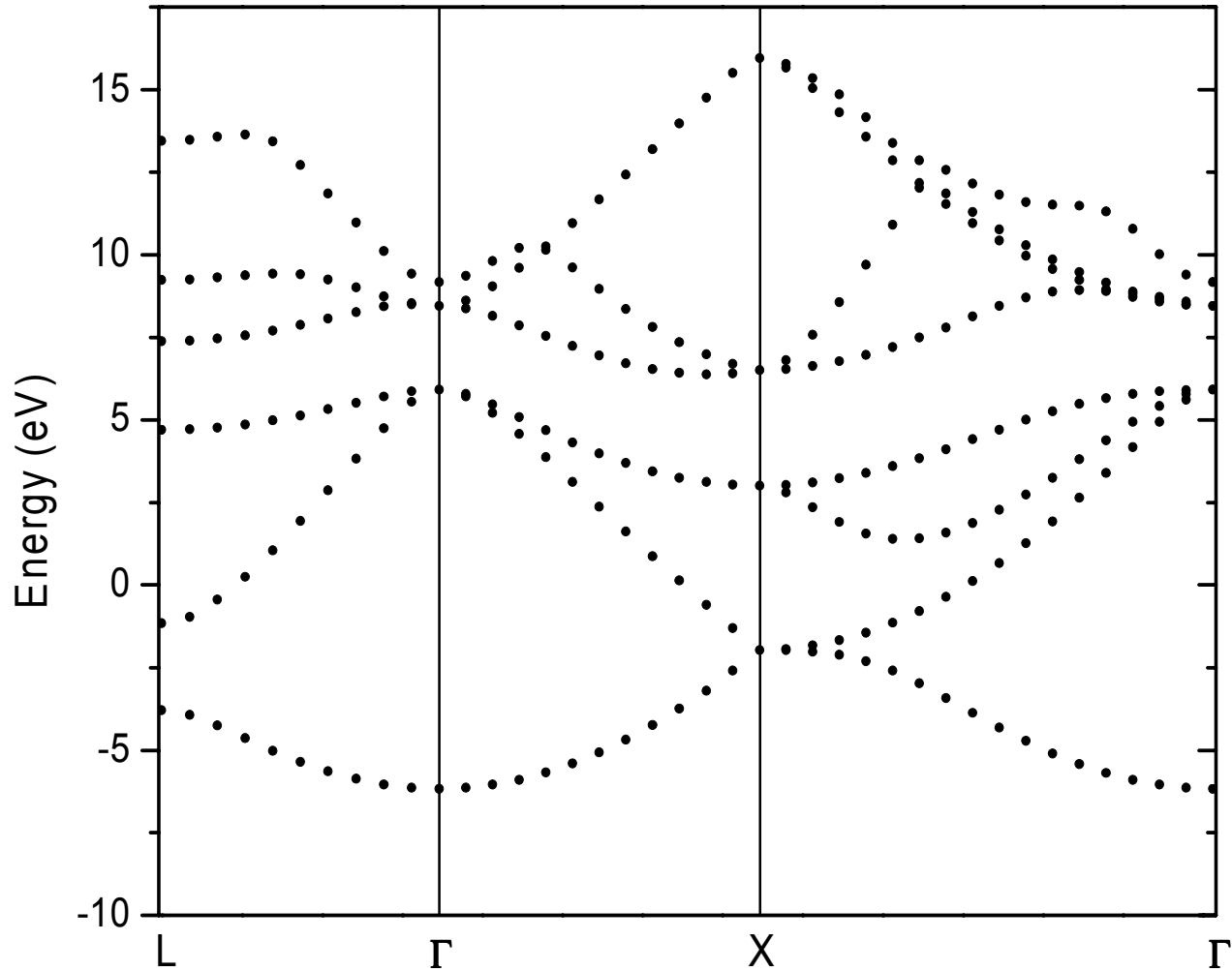


FIG. 3.14. The Brillouin zone for Γ_c^f . $\Gamma = (000)$; $X = (\frac{1}{2}0\frac{1}{2})$; $L = (\frac{1}{2}\frac{1}{2}\frac{1}{2})$; $W = (\frac{1}{2}\frac{1}{4}\frac{3}{4})$. K and U , though often referred to as points of symmetry, do not come within the definition of a point of symmetry as given in Definition 3.3.1, as they possess no more symmetry than the neighbouring lines Σ and S , respectively.

Si bands from `t35.out` (hand editing, short hack program, Origin plot)



Nice phonon band structure from t510_out.eps using program band2ps

