Phonon modeling in zinc-blende semiconductors

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Objective: Phonon modeling in zinc-blende semiconductors for the calculation of thermal properties.

Approach: **M**odified **VFF** → potential energy (U) → Dynamical matrix + boundary conditions → Phonons.

$$U_{MVFF} = U_{bb}+U_{bs}+U_{bb\text{-}bb}+U_{bb\text{-}bs}+U_{bs\text{-}bs}$$

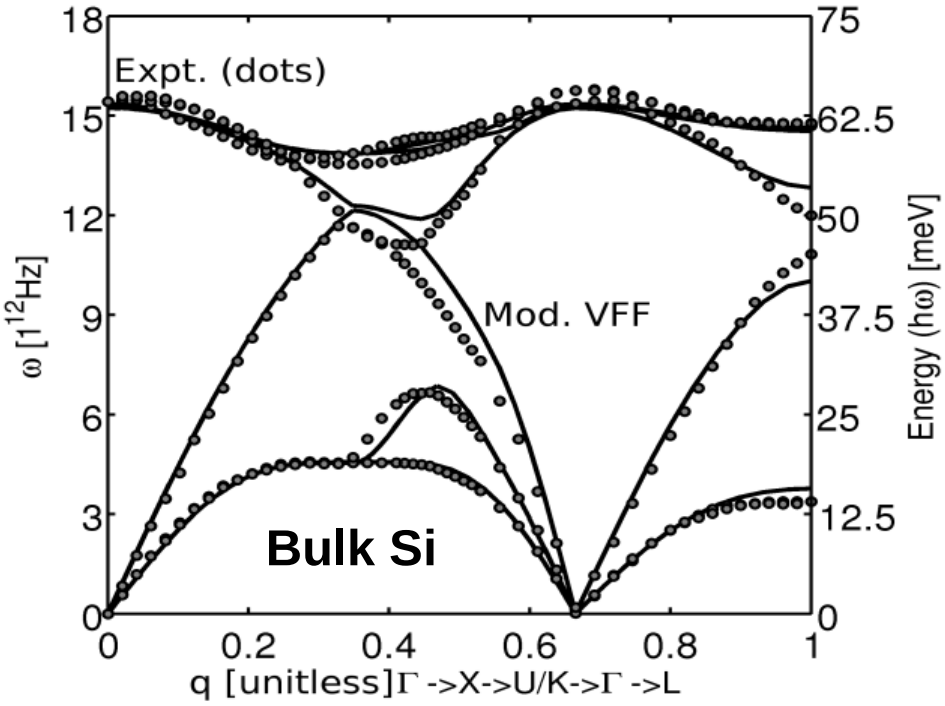
bb = bond-bending, bs = bond stretching

Impact:

(1) Good match with experimental bulk data.

(2) Method extended to free-standing nanowires.

Result.



Benchmarking of phonons in bulk Si.

Experimental data from: G. Nilsson and G. Nelin, Phys. Rev. B, 6 (10), 1972.