

## Alkali metal bulk moduli

$$\text{Electron density } n \equiv \frac{N_e}{V} = \frac{N_c Z}{a^3}$$

$N_c = \# \text{ atoms/cell} = 2$  for BCC

$Z = \text{valence} = 1$  for alkali metals

$a = \text{cubic lattice constant}$

$$\text{Fermi wavenumber } k_F = \sqrt[3]{3\pi^2 n}$$

$$\text{Fermi energy } E_F = \frac{\hbar^2}{2m} k_F^2 \quad m = \text{mass of electron (in metal)}$$

$$\text{Total electron energy } U = \frac{3}{5} E_F N_e \quad \text{density } U/V = \frac{3}{5} n E_F$$

$$\text{Pressure } P = -\frac{\partial U}{\partial V} = \frac{2}{3} \frac{U}{V} = \frac{2}{5} n E_F$$

$$\text{Bulk modulus } B = -V \frac{\partial P}{\partial V} = \frac{10}{9} \frac{U}{V} = \frac{2}{3} n E_F$$

element	$a(\text{\AA})$	$n(10^{28} \text{m}^{-3})$	$E_F(\text{eV})$	$B(\text{GPa})$	Expt. (low T)
Li	3.5	4.7	4.7	2.9	11
Na	4.2	2.7	3.3	9.2	6.3
K	5.2	1.4	2.1	3.2	3.1
Rb	5.6	1.2	1.9	2.3	2.5
Cs	6.0	0.9	1.6	1.5	1.6

Other metals less good - note mass in metal  $\neq$  mass in vacuum!