

Kittel 3.

The Lennard-Jones potential is given by

$$V(R) = \frac{A}{R^{12}} - \frac{B}{R^6}, \text{ but it's customary to write}$$

$$V(R) = 4\epsilon \left[ \frac{\sigma^{12}}{R^{12}} - \frac{\sigma^6}{R^6} \right], \text{ find } \epsilon, \sigma, \text{ show they}$$

are uniquely determined and explain the (significance) of this expression.

Trivially solving for  $\sigma, \epsilon$ :

$$\begin{cases} 4\epsilon \sigma^{12} = A \\ 4\epsilon \sigma^6 = B \end{cases}$$

$$\frac{A}{B} = \sigma^6, \quad \boxed{\sigma = \left(\frac{A}{B}\right)^{1/6}, \quad \epsilon = \frac{1}{4} \frac{B^2}{A}}$$

The advantage of this approach is that the single parameter  $\left(\frac{\sigma}{R}\right)^6$  allows one to easily see this potential algebraically is quadratic.

Kittel claims that  $\sigma, \epsilon$  can be obtained ~~for~~ from gas phase data, so these values are independent of the lattice type or any other solid-state properties, - specific