Kittel (8th Edition). Chapter 3. Problem 2.

$$u = \frac{1}{2}\sum_{\vec{r}\neq 0} 4\varepsilon\left[-\frac{1}{p^6}\left(\frac{\sigma}{R}\right)^6 + \frac{1}{p^{12}}\left(\frac{\sigma}{R}\right)^{12}\right]$$

$$= 2\varepsilon\left[\underbrace{-\sum_{\vec{r}\neq 0}\frac{1}{p^6}}_{A_6}\left(\frac{\sigma}{R}\right)^6 + \underbrace{\sum_{\vec{r}\neq 0}\frac{1}{p^{12}}}_{A_{12}}\left(\frac{\sigma}{R}\right)^{12}\right]$$

$$= 2\varepsilon\left[-A_6\left(\frac{\sigma}{R}\right)^6 + A_{12}\left(\frac{\sigma}{R}\right)^{12}\right]$$

$$\frac{\partial u}{\partial R} = 0 \Rightarrow 2\varepsilon\left[-A_6\frac{\partial}{\partial R}\left(\frac{\sigma}{R}\right)^6 + A_{12}\frac{\partial}{\partial R}\left(\frac{\sigma}{R}\right)^{12}\right] = 0$$

$$\Rightarrow 2\varepsilon\left[-6A_6\frac{\sigma^5}{R^6} + 12A_{12}\frac{\sigma^{11}}{R^{12}}\right] = 0$$

$$\Rightarrow -6A_6 + 12A_{12}\frac{\sigma^6}{R^6} = 0$$

$$\Rightarrow \frac{R^6}{\sigma^6} = \frac{2A_{12}}{A_6}$$

$$\Rightarrow R = \left(\frac{2A_{12}}{A_6}\right)^{\frac{1}{6}}\sigma$$

$$= \left(\frac{2\times 12.13188}{14.15392}\right)^{\frac{1}{6}}\sigma = 1.09017\,\sigma \qquad \text{for fcc.}$$

$$\left(\frac{2\times 9.11418}{12.2533}\right)^{\frac{1}{6}}\sigma = 1.06844\,\sigma \qquad \text{for bcc.}$$

$$\therefore \frac{u_{bcc}}{u_{fcc}} = \frac{2\varepsilon\left[-A_6\left(\frac{\sigma}{R}\right)^6 + A_{12}\left(\frac{\sigma}{R}\right)^{12}\right]_{bcc}}{2\varepsilon\left[-A_6\left(\frac{\sigma}{R}\right)^6 + A_{12}\left(\frac{\sigma}{R}\right)^{12}\right]_{fcc}} = \frac{\left[-12.2533\left(\frac{1}{1.06844}\right)^6 + 9.11418\left(\frac{1}{1.06844}\right)^{12}\right]}{\left[-14.45392\left(\frac{1}{1.09017}\right)^6 + 12.13188\left(\frac{1}{1.09017}\right)^{12}\right]}$$

$$= \frac{-8.236681 + 4.118281}{-8.610340 + 4.305240} = \underline{\underline{0.9566}}$$

Hence fcc structure is more stable than bcc structure.