Young's modulus meets Lennard-Jones

$$Y = -\frac{1}{r_0}\left(\frac{dF}{dr}\right)_{r=r_0}$$

But, $F = -\frac{dV}{dr}$ $\quad \therefore \quad Y = \frac{1}{r_0}\left(\frac{d^2V}{dr^2}\right)_{r=r_0}$

Also, $\quad V(r) = \varepsilon\left(\frac{r_0^{12}}{r^{12}} - \frac{2r_0^6}{r^6}\right)$

$$\frac{dV(r)}{dr} = \varepsilon\left(\frac{-12r_0^{12}}{r^{13}} + \frac{12r_0^6}{r^7}\right)$$

$$\frac{d^2V(r)}{dr^2} = \varepsilon\left(\frac{+156r_0^{12}}{r^{14}} - \frac{84r_0^6}{r^8}\right)$$

So $\quad \left|\frac{d^2V(r)}{dr^2}\right|_{r=r_0} = \varepsilon\left(\frac{156}{r_0^2} - \frac{84}{r_0^2}\right) = \frac{72\varepsilon}{r_0^2}$

$$\therefore \quad \boxed{Y = \frac{72\varepsilon}{r_0^3}}$$

Materials have a maximum breaking force, which occurs when the force applied to the atoms outweighs the attractive Lennard-Jones ~~potential~~ force between them, which occurs when $\frac{dF}{dr} = 0$

$$\frac{dF}{dr} = 0 \implies F = F_{max}$$

Can work out the distance, r_{max}, that this occurs at:

so use above expression lazily

$$0 = -\frac{dF}{dr} = \varepsilon\left(\frac{156r_0^{12}}{r^{14}} - \frac{84r_0^6}{r^8}\right) \implies r_{max} = \sqrt[6]{\frac{13}{7}}\,r_0$$

$F_{max} = \frac{2.64\varepsilon}{r\ldots}$