Potentials

(last modified 10/8/96)

The potential is often expressed as a series of one-body, two-body, three-body, and higher order potentials.

$$V = \sum_i V_1(r_i) + \sum_{i,j} V_2(r_{ij}) + \sum_{i,j,k} V_3(r_{ij}, r_{ik}, r_{jk}) + \cdots \tag{1}$$

The embedded atom method adds a potential term for each atom that is a function of the local density ρ_i around the atom,

$$V = \sum_{i<j} V_2(r_{ij}) + \sum_i F(\rho_i) \tag{2}$$

$$\rho_i = \sum_j f(r_{ij}) \tag{3}$$

($F(r)$ and $f(r)$ are empirical functions defined by these equations.)

The Stillinger-Weber potential for silicon has a three-body term that encourages tetragonal bond angles,

$$V_2(r) = (\frac{B}{r^4} - A)e^{\frac{1}{r-a}} \tag{4}$$

$$V_3(r_{ij}, r_{ik}, \theta_{jik}) = \lambda e^{\frac{\gamma}{r_{ij}-a} + \frac{\gamma}{r_{ij}-a}} \left[\cos(\theta) + \frac{1}{3}\right]^2 \tag{5}$$

where θ_{jik} is the angle between $\mathbf{r}_{ij}$ and $\mathbf{r}_{ik}$. These potential functions are set to zero for $r > a = 3.77$Å.

Please email any questions or corrections to shumway@uiuc.edu