Potential Details

0.1 SMA Potential (General Form)

The SMA potential is a sum of a repulsive part and an attraction potential that is a classical representation of the tight binding approach.

$$U_{coh} = U_{rep} + U_{el} \tag{1}$$

With r_{ij} being the inter-particle distance and N the total number of particles, we have

$$U_{el} = -\sum_{i=1}^{N} \left\{ \zeta_0^2 \sum_{j=1, j\neq i}^{N} exp[-2q(\frac{r_{ij}}{r_0} - 1)] \right\}^{1/2} \tag{2}$$

$$U_{rep} = \sum_{i=1}^{N} \epsilon_0 \sum_{j=1, j\neq i}^{N} exp[-p(\frac{r_{ij}}{r_0} - 1)] \tag{3}$$

0.2 Force Calculation

The MD simulation was done following the Velocity Verlet Time integration scheme. To determine the force for each inter-particle interaction, the derivative of the SMA potential was described as

$$F(r_{ij}) = -\frac{dU_{coh}}{dr_{ij}} \tag{4}$$

Using

$$u = -p(\frac{r_{ij}}{r_0} - 1)$$

$$v = -2q(\frac{r_{ij}}{r_0} - 1)$$

We have

$$\frac{dU_{coh}}{dr_{ij}} = \epsilon_0 \left[\sum_{j\neq i} exp(u) \frac{du}{dr_{ij}} \right] - \left[\frac{\sum_{j\neq i} \frac{\zeta_0^2}{2} exp(v) \frac{dv}{dr_{ij}}}{\left(\sum_{j\neq i} \zeta_0^2 exp(v) \right)^{\frac{1}{2}}} \right] \tag{5}$$

0.3 Modified Potential (To code)

With r_{ij} being the inter-particle distance and N the total number of particles, we have

$$U = \frac{\epsilon}{2} \sum_{i=1}^{N} \left[A \sum_{j=1, j\neq i}^{N} exp[-p(\frac{r_{ij}}{r_0} - 1)] - \left\{ \sum_{j=1, j\neq i}^{N} exp[-2q(\frac{r_{ij}}{r_0} - 1)] \right\}^{1/2} \right] \tag{6}$$

0.4 Interaction Parameters

The parameters ϵ,A, p, q and r_0 for Ni as used in the simulation are:

ϵ	A	p	q	r_o
1.51	17.8	9.62	1.45	9.44