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

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

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

More details and other parameters for the SMA potential to be found here [1].

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 or Ni (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 for Ni as used in the simulation are $\epsilon = 1.0$, $A = 0.03514$, $p = 17.0$, $q = 1.19$,$r_o = 1$ and unit of time $t_o = \sqrt{mr_o^2/\epsilon}$

References

[1] Y.Li, E.B.B, and D.A. Papa, Structure and Dynamics of Alkali Metal Clusters and fission of highly charged clusters, Phys. Rev. B, (57) 15519, 1998 https://journals.aps.org/prb/pdf/10.1103/PhysRevB.57.15519