Examination MD Simulation for Microscale Heat Transfer

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For a substance expressed with Lennard-Jones (12-6) potential

$$\phi(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \qquad (1)$$

answer the following questions.

(a) Derive the non-dimensional forms for following variables.

- Temperature T
- Force F
- Pressure P
- Surface tension γ
- Thermal conductivity λ

(b) Calculate the pair separation at which the Lennard-Jones potential is a minimum.

(c) Guess why “4” is used in equation (1). Isn’t is simpler to define the potential as

$$\phi(r) = \varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right].$$

(d) Use the Newton’s second law to show that in terms of the potential parameters ε and σ, the unit of time is $\sigma\sqrt{m/\varepsilon}$, where m is the mass of one atom.

(e) The long-range correction for potential energy E_p is expressed as

$$\frac{E_p}{N} = \frac{\tilde{E}_p}{N} + E_{pLR}$$

$$E_{pLR} \approx 2\pi\rho\int_{r_c}^{\infty}\phi(r)r^2 dr$$

Derive the following expression for Lennard-Jones potential.

$$E^*_{pLR} = \frac{8\pi\rho^*}{3(r_c^*)^3}\left(\frac{1}{3(r_c^*)^6} - 1\right)$$

(f) Consider two molecules at $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$. Probe that the force $\mathbf{F}_i = -\nabla_i\phi$ acting on molecule i is expressed as

$$\mathbf{F}_i = 24\varepsilon\left[2\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]\frac{\mathbf{r}_{ij}}{r_{ij}^{\ 2}} \qquad \text{where } \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j \text{ and } r_{ij} = \left|\mathbf{r}_{ij}\right|.$$