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$$\begin{aligned}
T^* &= k_B T / \epsilon \\
\rho^* &= \rho \sigma^3 \\
\kappa^* &= \kappa \sigma^2 \sqrt{m} / (k_B \sqrt{\epsilon}) \\
t^* &= t \sqrt{\epsilon} / (\sigma \sqrt{m})
\end{aligned}$$

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$$\begin{aligned}
\vec{w}^2 &= (\alpha \vec{r} + \beta \vec{b})^2 \\
&= \alpha^2 r^2 + \beta^2 b^2 + 2\alpha\beta \vec{r} \cdot \vec{b} \\
&= \alpha^2 r^2 + (1 - \alpha \frac{\vec{r} \cdot \vec{b}}{b^2})^2 b^2 + 2\alpha(1 - \alpha \frac{\vec{r} \cdot \vec{b}}{b^2}) \vec{r} \cdot \vec{b} \\
&= \alpha^2 r^2 + (1 + \alpha^2 \frac{(\vec{r} \cdot \vec{b})^2}{b^4} - 2\alpha \frac{\vec{r} \cdot \vec{b}}{b^2}) b^2 + 2\alpha(1 - \alpha \frac{\vec{r} \cdot \vec{b}}{b^2}) \vec{r} \cdot \vec{b} \\
&= \alpha^2 r^2 + b^2 - \alpha^2 \frac{(\vec{r} \cdot \vec{b})^2}{b^2} \\
&= b^2 + \frac{|\alpha|^2}{b^2} (r^2 b^2 - (\vec{r} \cdot \vec{b})^2)
\end{aligned}$$

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In our calculations, the standard deviation of temperature in a certain slab  $m$  is expressed as

$$\sigma_{m,s} = \sqrt{\frac{\sum_{i=1}^{\mathcal{N}} (T_{m,i} - \bar{T}_m)^2}{\mathcal{N} - 1}} \quad (1)$$

where  $\bar{T}_m$  is the average value for measurements  $T_{m,i}$  and  $\mathcal{N}$  represents the total number of measurements. The standard deviation of the averaged value  $\bar{T}_m$ , therefore, is given by

$$\sigma_m = \frac{\sigma_{m,s}}{\sqrt{\mathcal{N}}} \quad (2)$$

$$= \sqrt{\frac{\sum_{i=1}^{\mathcal{N}} (T_{m,i} - \bar{T}_m)^2}{\mathcal{N}(\mathcal{N} - 1)}} \quad (3)$$

With a set of data  $(\bar{T}_m, \sigma_m)$  where  $m$  goes from 0 to  $N-1$  in our model, we do the fit to the cosine function to determine and fitting parameter of amplitude, which is  $\Delta T$  in Eq.(1). The standard deviation of  $\Delta T$  is determined at the same time. Then by using Eq.(2) we can get a relation between  $\sigma_{\Delta T}$  and  $\sigma_{\kappa_{\text{eff}}}$ , which is

$$\frac{\sigma_{\kappa}}{\kappa_{\text{eff}}} = \frac{\sigma_{\Delta T}}{\Delta T} \quad (4)$$

Thus  $\sigma_{\kappa_{\text{eff}}} = \kappa_{\text{eff}} \sigma_{\Delta T} / \Delta T$  gives the standard deviation of  $\kappa$ .

## Liquid

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Cutoff distance for LJ potential  $3.0\sigma$

Width of slab  $d = a = 5.31\text{\AA}$ , 1.56 in reduced units with LJ constant  $\sigma$  for Argon  $3.405\text{\AA}$  The simulations are conducted on supercells of  $6 \times 6 \times N$  cubic conventional cells with  $N$  a parameter for approaching the bulk limit. This 6 by 6 simulation proves reasonable from comparing the behaviour of  $\kappa(q)$  around the  $q = 0$  with that predicted by Debye Model and in order to do this, we treated the solution of Boltzmann equation in two different ways.

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Time

The LJ unit, a unit time for Argon should be  $\tau_{LJ}=2.16\text{ps}$

For short sample time step is  $\Delta t^* = 6.965 \times 10^{-3}$ , while for longer sample  $\Delta t^* = 2 \times 6.965 \times 10^{-3}$

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$$X = [\delta - (v_H^2 - v_C^2)] \cdot \frac{\delta}{|\vec{v}_H + \vec{v}_C|^2} \cdot \frac{b^2}{b^2 r^2 - (\vec{b} \cdot \vec{r})^2}$$

For safety in evolutions, we'd better keep  $X$  negative. As shown in Eqs.(10) the last two terms are positive so  $\delta - (v_H^2 - v_C^2) = 2\Delta/m - (v_H^2 - v_C^2)$  dominates. It is found in tests that  $v_H^2 - v_C^2$  sometimes touches the ground of 3(in L-J reduced units), so if  $W$  were set to be 480 in this case, for instance, we would soon find errors in the data. One may insist on a  $W$  which is much smaller than 60 to enable inputs with larger amplitudes for the simple reason that large imposes converge much faster. However, this proves unnecessary: it has been shown in Muller-Plathe's method that validity of linear response theory breaks down for large variation with  $W = 15$ , which is parallel to the impose with  $\dot{e} = 10.120$  in our theory. So even if, with lower  $W$  and larger input amplitude, there is nothing wrong with the calculation of vector  $\vec{w}$ , it is meaningless to do calculations of this kind without the validity of linear response theory. It is been tested that  $W = 60$  does not work for  $\dot{e} = 10.120$ , therefore, our choice of  $W$  seems quite reasonable.

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Time step  $\Delta t^* = 6.965 \times 10^{-3}$  and it is very interesting that this is a guess from dimension argument.

We choose crystal constant  $a$  as the width of the slab so we can keep 144 atoms in each slab. By doing this, we can ensure a quite large  $(v_H^2 - v_C^2)$

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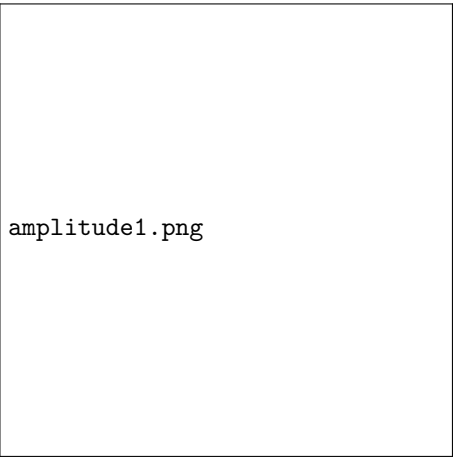
Here, the critical parameter for the MullerPlathe is  $W=120$  while for the new algorithm is  $e=1.265$ , and to ensure a solution for  $X$ ,  $W$  is chosen to be 60.

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## Crystal

- 08/11 In experiment,

$$\kappa^* = \kappa \times 52.943$$



amplitude1.png

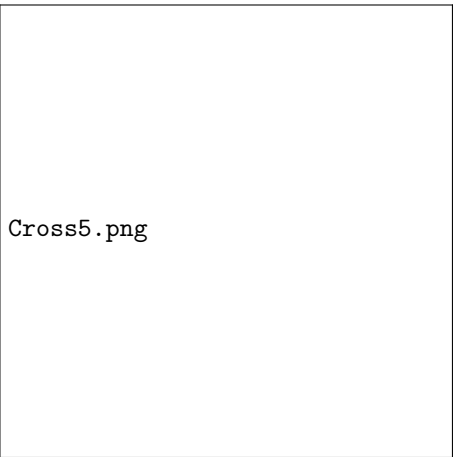
for crystal,  $\kappa = 0.31W/(m \cdot K)$ ,  $\kappa^* = 16.41 - - - - - 77K$

for liquid,  $\kappa = 0.1324W/(m \cdot K)$ ,  $\kappa^* = 7.01 - - - - - 85K$

CRC Handbook of Chemistry and Physics, 85th Edition, David R. Lide (Editor), CRC Press

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I changed the x axis so this figure is more reader-friendly.



Cross5.png

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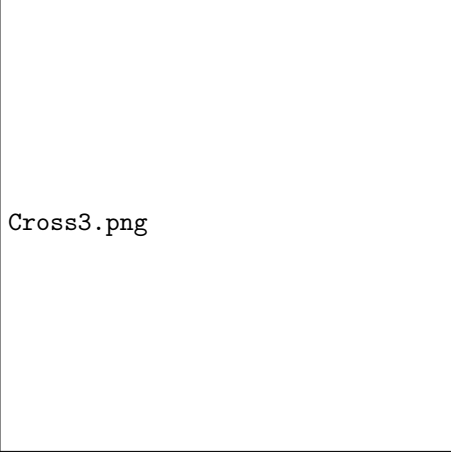
The temperature for simulation on crystal is 80 K, which is 0.66 in LJ unit and the amplitude of the sine function in temperature profile is 0.03 in LJ unit.

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N3 is 12,16,20,28,32,36,56,64,72,120,128,136 in my simulation.

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summing over Brillouin Zone, the length of the sample is  $500a=500d$ , the ratio is divided by the  $\kappa(192)$



## Extrapolation

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Temperature approximately 80K, 0.66 in LJ unit, with the scaling  $\epsilon/k_B = 119.6K$ , I keep the temperature variance 0.03 during the simulation(LJ unit) to keep my system efficient. We run those systems at constant temperature.

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$$\frac{\kappa(q)}{\kappa_D} = \frac{3-p}{N} \cos^2(qd/2) \sum_{\vec{Q}} \frac{Q_x^2}{\vec{Q}^2} \left(\frac{Q_D}{Q}\right)^p \cdot F(q, u)$$

$Q_D = (6\pi^2(N/V))^{1/3}$  in the case of fcc  $Q_D = (3/\pi)^{1/3} \frac{2\pi}{a} = 0.985 \frac{2\pi}{a}$

$Q_x$  is the projection of  $\vec{Q}$  in  $(1,1,\bar{1})$  direction.