Constant Temperature Boundary Conditions with Phantom Molecules (Langevin Method)

Introduction

Most heat transfer simulations need to use the constant temperature solid wall boundary condition. The simple velocity scaling is often applied to three crystal layers of harmonic molecules. Since the velocity scaling is too artificial, the following phantom technique [1-5] is recommended. Phantom molecules model the infinitely wide bulk solid kept at a constant temperature T with the reasonable heat conduction characteristics.

An example of the configuration of phantom molecules for a harmonic fcc solid system is shown in Fig. 1. The surface is fcc (111). In this case 3 layers are real molecules. A phantom molecule is connected to each real molecule at the bottom layer by the special spring. It is also connected with fixed molecule (fixed frame) through the special spring and the special damper. Furthermore, phantom molecules are excited with the random force.

The connections are summarized as follows:

Between a phantom molecule and a real molecule
    Spring of vertical 2k and horizontal 0.5k
Between a phantom molecule and a fixed molecule (fixed frame)
    Spring of vertical 2k and horizontal 3.5k + damper

Details of springs, dampers, and random force are following.

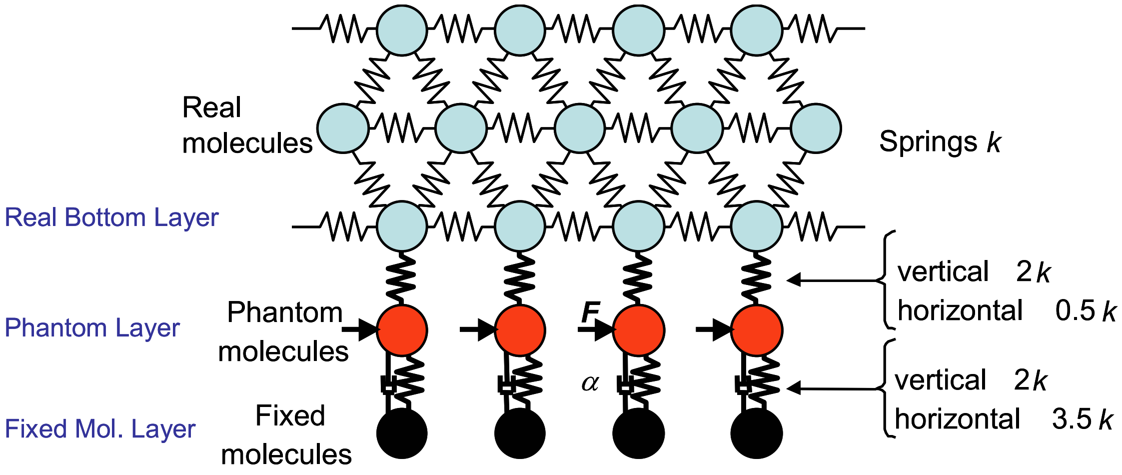

Figure 1 Constant temperature solid wall with phantom molecules.

The connection between a real molecule and a phantom molecule

A phantom molecule situates just below a real molecule at the bottom layer. Let's assume a special spring between a real molecule and a phantom molecule. The phantom molecules must replace the layers of real molecules.

Let's focus on a real molecule on the bottom layer. For this real molecule, phantom molecules should behave like real molecules. It should be connected to 3 molecules at the phantom level. This real molecule and 3 molecules are in the tetrahedral position. There are 3 springs between a real molecule and 3 molecules at the phantom level. Effect of these 3 molecules must be expressed by the special spring and a one phantom molecule. Imagine a small displacement dz of real molecule in vertical direction.

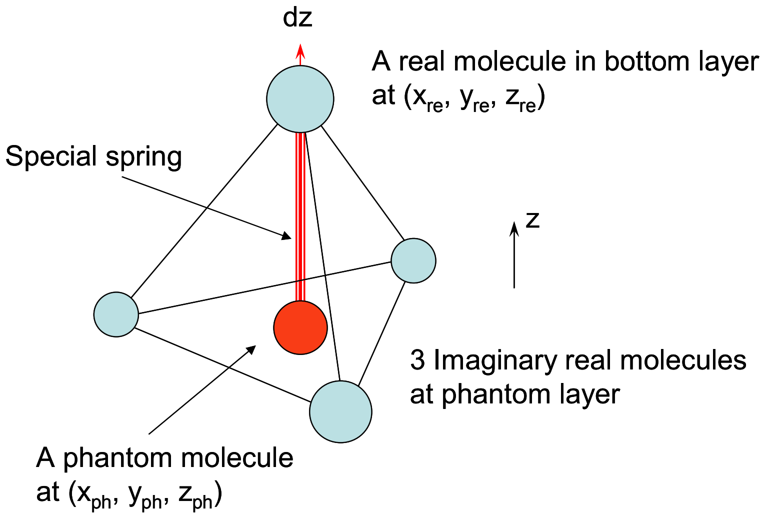

Figure 2 Connection between a real molecule and a phantom molecule

For a spring:

The increase in spring length is $\sqrt{2/3}dz$.

The force in spring direction is $k\sqrt{2/3}dz$.

The force component in z direction is $\sqrt{2/3}k\sqrt{2/3}dz = \frac{2}{3}k\ dz$

There are symmetric 3 springs. Force components other than z direction cancel each other. Then, the total spring force due to a vertical displacement dz is $2k\ dz$. Hence, the vertical spring constant for the special spring is $2k$.

If you assume horizontal small displacements dx or dy, the similar discussions result the strength of horizontal spring constant of $0.5k$. It should be noted that this horizontal spring applies to 2 directions, x and y.

Let's define that a real molecules coordinate is (x_{re}, y_{re}, z_{re}) and a phantom molecules coordinate is (x_{ph}, y_{ph}, z_{ph}). Then, the special spring gives forces as

$$f_x = 0.5k(x_{re} - x_{ph})$$

$$f_y = 0.5k(y_{re} - y_{ph})$$

$$f_z = 2k(z_{re} - z_{ph})$$

Connection between a phantom molecule and a fixed molecule

Now, the special spring between a phantom molecule and a fixed molecule should replace 9 real springs. A real molecule at the phantom layer should be connected with 6 springs in the same layer and 3 springs in the fixed molecule layer. Since there is no springs between phantom molecules, effect of these all 9 springs should be included in the special spring between a phantom and a fixed molecule. From the same discussion as before, the spring constants are 2k in vertical direction and 3.5 k in horizontal direction. This extra 2k is for 6 springs in the same layer.

Let's define that a phantom molecules coordinate is (x_{ph}, y_{ph}, z_{ph}) and a fixed molecule coordinate is (x_{fix}, y_{fix}, z_{fix}). Then, the force to a phantom molecule from special spring is

$$f_x = -3.5k(x_{ph} - x_{fix})$$
$$f_y = -3.5k(y_{ph} - y_{fix})$$
$$f_z = -2k(z_{ph} - z_{fix})$$

In addition to the harmonic spring, dampers are connected between a phantom molecules and a fixed molecule with the damping coefficient of

$$\alpha = m\frac{\pi}{6}\omega_D = m\frac{\pi}{6}\frac{k_B\theta}{\hbar}$$

where, ω_D is the Debye frequency, and θ called Debye temperature. In the case of platinum, as an example, Debye temperature θ is 240 K and $\alpha = 5.18\times10^{-12}$ kg/s.

Each phantom molecule is excited by the random force *F* of Gaussian distribution with the standard deviation

$$\sigma_F = \sqrt{\frac{2\alpha k_B T_C}{\Delta t}}$$

from 3 directions in each time step of Δt.

The energy flux to the calculation system can be accurately calculated by integrating the exciting force and the damping force applied to phantom molecules [4, 5]. Then, the expected amount of energy gain by this random force is the same as the energy lost by the damper when the temperature is at the desired temperature T_c.

References

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