Phononic friction and heat transfer between nanoscale water flow and graphene layers

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Calculations are given of the friction coefficient and the heat transfer coefficient at the interface between water and a system of graphene layers within the framework of a model in which the interaction between fluctuating displacements of water and graphene surfaces was described by the Lennard-Jones potential and the electrostatic potential. The friction coefficient and the heat transfer coefficient increase with an increase in the number of graphene layers and reach saturation for \( N > 10 \), which is attributed to an increase in the phonon transmission coefficient across the interface and a finite phonon mean free path in the direction perpendicular to the surface.

PACS: 44.40.+a, 63.20.D-, 78.20.Ci

I. INTRODUCTION

Friction at water-carbon interface in nanoscale channel has received recently significant attention due to its relevance in nanoscale systems\(^1\). Experiments and simulations have found that water moves practically without friction through carbon nanotubes\(^2-5\). These observations have stimulated active studies in nanotube-based membranes for applications including desalination, nano-filtration and energy harvesting\(^6-11\). However, the mechanism of water-carbon friction remains not well understood\(^12-16\).

The fluctuations inside media produce a fluctuating electromagnetic field which is responsible for Casimir forces. At non-equilibrium conditions when there is temperature difference between media or media are moving relative to each other the same fluctuating electromagnetic field produces radiative heat transfer and Casimir friction\(^17,18\). In the near field, for the separation between media smaller than the characteristic thermal wavelength \( \lambda_T \) (\( \lambda_T = c\hbar/k_BT \), at room temperature \( \lambda_T \sim 10\mu\text{m} \)) radiative heat transfer and Casimir friction are enhanced by many orders of the magnitudes due to the contribution from the evanescent electromagnetic waves. However, in an extreme near-field, when the separation between media \( \sim 1\text{nm} \), the van der Waals and electrostatic interaction between fluctuating surface displacements produce phonon heat transfer, dominated by acoustic waves, which exceeds radiative heat transfer\(^19-22\).

Here we present a general theory of phononic friction between closely spaced media which is a generalization of our theory of phononic heat transfer\(^22\). In our theory, friction arises due to the interaction between surface displacements experiencing thermal and quantum fluctuations. The theory is applied to study friction between water flow and graphene layers. We calculate numerically friction coefficient and heat transfer coefficient in dependence on the number of graphene layers. The theory of the phononic friction was also applied by us to calculate the friction coefficient for the interface between two gold surfaces\(^29\).

FIG. 1: Schematic view of water flow and graphene layers. Thermal fluctuations of surface displacements of water \( u_d \) and graphene sheet \( u_g \) produce fluctuating stresses acting on the surfaces due to the van der Waals and electrostatic interaction. These fluctuating stresses are responsible for the phononic friction and heat transfer between water flow and graphene layers.
II. THEORY

A schematic view of our model, which consists of a water block and a system of graphene layers, is shown in Fig. 1. Calculations of the Kapitza resistance within a similar model using molecular dynamics methods showed that the results depend on the number of graphene layers, but do not depend on the thickness of the water block when it exceeds 2nm. In our calculations, the water block was considered in the isotropic continuum model, and the graphite sheet was considered as an elastic membrane. A schematic view of our model is shown. It consists of a water block and a system of graphene layers. Graphene sheet and water are considered as an elastic membrane and an elastic isotropic continuum medium, respectively. The interlayer carbon interactions were modelled by pairwise Lennard-Jones (L.-J) potential

\[ V_{ij} = 4\varepsilon_{ij} \left( \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right) \]

using the parameters from Girifalco et al. The carbon-water interaction were modelled by L.-J potentials with parameters taken from work of Werden et al. Values of L.-J parameters are provided in Table I.

| Pair       | \( \sigma (\text{Å}) \) | \( \varepsilon (\text{kJ/mol}) \) |
|------------|-----------------|-----------------|
| C-O        | 3.190           | 0.3920          |
| C-C        | 3.414           | 0.2313          |
| C-H        | 0               | 0               |

Thermal fluctuations of surface displacements of water \( u_d \) and graphene \( u_g \) will create surface stresses. In the rest reference frame of graphene (\( K \) frame), in which water moves at velocity \( v \), a stress acts on the graphene surface \[ \sigma_g(x, t) = -K_0 u_g(x, t) + \int d^3x_1 K(x - x_1) u_d(x_1 - vt, t), \] (2)

and in the co-moving to water flow reference frame (\( K' \) frame) on water surface acts stress

\[ \sigma_d(x', t) = -K_0 u_d(x', t) + \int d^3x_1 K(x' - x_1') u_g(x_1' + vt, t). \] (3)

In the case of L.-J potential

\[ K_0 = 30\pi n_O n_C \varepsilon_{C-O} d_0^4, \quad K((x - x_1)) = \frac{4K_0}{5\pi} \left\{ \frac{2\sigma_{C-O}^{12}}{[|x - x_1|^2 + d_0^4]^7} - \frac{\sigma_{C-O}^6}{[|x - x_1|^2 + d_0^4]^4} \right\} \]

where \( d_0 = (2/5)^{1/6}\sigma_{C-O} = 2.738\text{Å} \) is the equilibrium distance between water and graphene, \( n_O = 3.34 \cdot 10^{28}\text{m}^{-3} \) is the concentration of oxygen atoms in water, \( n_C = 3.85 \cdot 10^{19}\text{m}^{-2} \) is the concentration of carbon atoms in graphene sheet. As a result of the Fourier transformation

\[ u_i(x, t) = \int \frac{d\omega}{2\pi} \int \frac{d^2q}{(2\pi)^2} u_i(\omega, q) e^{-i\omega t + iq \cdot x}, \] (4)

Eqs. (2) and (3) take the form

\[ \sigma_g(\omega, q) = -K_0 u_g(\omega, q) + K u_d(\omega', q), \] (5)

\[ \sigma_d(\omega', q) = -K_0 u_d(\omega', q) + K u_g(\omega, q), \] (6)

where \( \omega' = \omega - q_x v \) is the Doppler shifted frequency,

\[ K = \frac{q^3 d_0^6 K_0}{12} \left[ \frac{q^3 d_0^6 K_6(qd_0)}{192} - K_3(qd_0) \right], \] (7)
where the value of the following integral was used:

\[
\int d^2 \mathbf{x} \frac{e^{i \mathbf{q} \cdot \mathbf{x}}}{(q^2 + d^2)^{\mu+1}} = 2\pi \int_0^\infty J_0(qr) r dr = \frac{\pi}{2\mu+1} \left( \frac{q}{d} \right)^\mu \frac{K_\mu(qd)}{\Gamma(\mu+1)}
\]  
(8)

where \( K_\mu(z) \) is the Bessel function of the second kind and order \( \mu \) (see Ref. 27).

The surface displacements due to thermal and quantum fluctuations are determined by 19,22

\[
u_g(\omega) = u_g^f(\omega) + M_g(\omega)[-K_0 u_g(\omega) + K u_d(\omega')],
\]  
(9)

\[
u_d(\omega') = u_d^f(\omega') + M_d(\omega')[-K_0 u_d(\omega') + K u_g(\omega)],
\]  
(10)

where according to the fluctuation-dissipation theorem, the spectral density of fluctuations of the surface displacements is determined by 28

\[
\langle |u_i^f|^2 \rangle = \hbar \text{Im} M_i(\omega, q) \coth \frac{\hbar \omega}{2k_B T_i}
\]  
(11)

where \( \langle \cdots \rangle \) denotes thermal average, \( M_i \) is the mechanical susceptibility for surface \( i \): \( u_i = M_i \sigma \). A potential difference between graphene and electrode (see Fig. 1) induces the surface charge densities on graphene \( \sigma_g = E_0/4\pi \) and water \( \sigma_w = -\sigma_s(\varepsilon_0 - 1)/\varepsilon_0 \approx \sigma_g \) where \( E_0 \) is the electric field in the vacuum gap between graphene and water induced by voltage and \( \varepsilon(0) \approx 80 \) is the static dielectric constant for water. In the case of electrostatic interaction between fluctuating displacements of charged surfaces of graphene and water19,21,

\[
K_0 = \frac{E_0^2}{4\pi} q \frac{1 + e^{-2q|d|}}{1 - e^{-2q|d|}},
\]  
(12)

\[
K = \frac{E_0^2}{2\pi} q e^{-q|d|}.
\]  
(13)

From Eqs. (9) and (10)

\[
u_g(\omega) = \frac{(1 + K_0 M_d(\omega') u_g^f(\omega) + K M_g(\omega) u_d(\omega'))}{(1 + K_0 M_g(\omega))(1 + K_0 M_d(\omega'))} - K^2 M_g(\omega) M_d(\omega'),
\]  
(14)

\[
u_d(\omega') = \frac{(1 + K_0 M_g(\omega) u_d^f(\omega') + K M_d(\omega')) u_g(\omega)}{(1 + K_0 M_g(\omega))(1 + K_0 M_d(\omega'))} - K^2 M_g(\omega) M_d(\omega'),
\]  
(15)

The heat generated by fluctuating stresses in water and graphene system are determined by

\[
\left( \begin{array}{c} \dot{Q}_g \\ \dot{Q}_d \end{array} \right) = \int \frac{d\omega}{2\pi} \int \frac{d^2 \mathbf{q}}{(2\pi)^2} \left( \begin{array}{c} -i\omega < u_g(\omega)\sigma_g(\omega) > \\ -i\omega' < u_d(\omega')\sigma_d(\omega') > \end{array} \right) =
\]

\[
= 2\hbar \int \frac{d\omega}{2\pi} \int \frac{d^2 \mathbf{q}}{(2\pi)^2} \left( \begin{array}{c} \omega \\ -\omega' \end{array} \right) \frac{K^2 \text{Im} M_g(\omega) M_d(\omega') [n_d(\omega') - n_g(\omega)]}{| (1 + K_0 M_g(\omega))(1 + K_0 M_d(\omega')) - K^2 M_g(\omega) M_d(\omega') |^2}
\]  
(16)

where \( n_i(\omega) = [\exp(\hbar \omega/k_B T_i) - 1]^{-1} \). The friction force can be calculated from equation 18

\[
f_x v = \dot{Q}_g + \dot{Q}_d.
\]  
(17)

From Eqs. (3) and (17) the friction force 29

\[
f_x = 4\hbar \int \frac{d\omega}{2\pi} \int \frac{d^2 \mathbf{q}}{(2\pi)^2} g_x \frac{K^2 \text{Im} M_g(\omega) \text{Im} M_d(\omega')}{| (1 + K_0 M_g(\omega))(1 + K_0 M_d(\omega')) - K^2 M_g(\omega) M_d(\omega') |^2} |n_d(\omega') - n_g(\omega)|.
\]  
(18)
To linear order on velocity $v$ the friction force $f_z = \gamma v$ where at $T_g = T_d = T$ the phonon friction coefficient

$$
\gamma_{ph} = \frac{\hbar^2}{8\pi^2 k_B T} \int_0^\infty \frac{d\omega}{\sinh^2(h\omega/2k_B T)} \int_0^\infty dq^3 \frac{K^2 \text{Im} M_g(\omega)\text{Im} M_d(\omega)}{1 + K_0 M_g(\omega) + K_0 M_d(\omega) - K^2 M_g(\omega)M_d(\omega)}.
$$

At $v = 0$ the heat flux due to the phonon tunneling

$$
J(T_g, T_d) = \dot{Q}_g = -\dot{Q}_d = 4\hbar \int_0^\infty \frac{d\omega}{2\pi} \int \frac{d^2 q}{(2\pi)^2} \frac{K^2 \text{Im} M_g(\omega)\text{Im} M_d(\omega)[n_d(\omega) - n_g(\omega)]}{(1 + K_0 M_g(\omega) + K_0 M_d(\omega) - K^2 M_g(\omega)M_d(\omega))^2}.
$$

and the heat transfer coefficient

$$
\alpha(T) = \lim_{\Delta T \to 0} \frac{J(T, T + \Delta T)}{\Delta T} = \frac{\hbar^2}{4\pi^2 k_B T^2} \int_0^\infty \frac{d\omega}{\sinh^2(h\omega/2k_B T)} \int_0^\infty dq^3 \frac{K^2 \text{Im} M_g(\omega)\text{Im} M_d(\omega)}{|1 + K_0 M_g(\omega) + K_0 M_d(\omega) - K^2 M_g(\omega)M_d(\omega)|^2}.
$$

III. SURFACE MECHANICAL SUSCEPTIBILITY FOR WATER AND SYSTEM OF GRAPHENE LAYERS

In the elastic continuum model for isotropic medium the surface displacement under the action of external mechanical stress $u = M\sigma_{zz}^{ext}$ where mechanical susceptibility $^{31}$

$$
M_d = \frac{i}{\rho \omega^2} \left( \frac{\omega}{c_t} \right)^2 \frac{p_l(\omega)}{S(\omega, \omega)},
$$

where

$$
S(\omega, \omega) = \left[ \left( \frac{\omega}{c_t} \right)^2 - 2q^2 \right]^2 + 4q^2 p_l p_l,
$$

$$
p_l = \left[ \left( \frac{\omega}{c_t} \right)^2 - q^2 + i0 \right]^{1/2},
$$

$$
p_l = \left[ \left( \frac{\omega}{c_t} \right)^2 - q^2 + i0 \right]^{1/2},
$$

where $\rho$, $c_l$, and $c_t$ are the mass density of the medium, the velocity of the longitudinal and transverse acoustic waves. For water $c_t = 0$, $c_l = 1500m/s$ and $M_d$ is reduced to the form

$$
M_d = \frac{i p_l}{\rho \omega^2}.
$$

One graphene layer can be considered as an elastic membrane for which the mechanical susceptibility related with out-of-plane displacement $^{22}$

$$
M_{ls} = \frac{1}{\kappa q^4 - \rho \omega^2 - i\omega \rho \gamma},
$$

where the bending stiffness of graphene $\kappa \approx 1eV$, $\rho = 7.7 \cdot 10^{-7}kg/m^2$ is the surface mass density of graphene, $\gamma$ is the damping constant for flexural motion of graphene which was estimated in Ref $^{25}$ as

$$
\gamma = \frac{\omega T}{100T_{RT}}
$$

where $T_{RT} = 300K$ is the room temperature. For number of interacting graphene layers $N \geq 2$ the mechanical susceptibility can be found from equations

$$
(\Delta - C)u_1 + Cu_2 = -\sigma_0 e^{-i\omega t} q \cdot x
$$
\[ \text{Cu}_1 + (\Delta - 2C)\text{Cu}_2 + \text{Cu}_3 = 0 \]

\[ \text{Cu}_{N-2} + (\Delta - 2C)\text{Cu}_{N-1} + \text{Cu}_N = 0 \]

\[ \text{Cu}_{N-1} + (\Delta - C)\text{Cu}_N = 0 \]  \hfill (26)

where \( \Delta = \rho \omega^2 - \kappa q^4 + i \omega \eta(\omega) \), for the L.-J. interaction between graphene layers the spring constant for interlayer interaction

\[ C = 8 \pi n_e^2 e^{-c-c} \left[ 11 \left( \frac{\sigma_{c-c}}{a} \right)^{12} - 5 \left( \frac{\sigma_{c-c}}{a} \right)^{6} \right] = 1.16 \cdot 10^{20} \text{Nm}^{-3} \]  \hfill (27)

where \( a = 3.35 \text{Å} \) is the interlayer separation, \( n_c = 3.85 \cdot 10^{19} \text{m}^{-3} \) is the concentration of carbon atom in graphene sheet. The solution of the system of Eqs. (26) can be written in the form

\[ u_n = C_1 \lambda^{n-1} + C_2 \lambda^{-n+1} \]  \hfill (28)

where

\[ \lambda = 1 - \frac{\Delta}{2C} + \sqrt{\left( \frac{\Delta}{2C} - 1 \right)^2 - 1} \]  \hfill (29)

is the root of equation

\[ \gamma^2 - 2 \left( 1 - \frac{\Delta}{2C} \right) \gamma + 1 = 0 \]  \hfill (30)

for which \(|\gamma| < 1\). The constants \( C_1 \) and \( C_2 \) are determined by equations which are obtained after substitution of Eq. (28) in system (26)

\[ [\Delta + C(\lambda - 1)]C_1 + [\Delta + C(\frac{1}{\lambda} - 1)]C_2 = -\sigma_0 e^{-i\omega + iq \cdot \mathbf{x}} \]  \hfill (31)

\[ \lambda^{2(N-1)} \left[ \Delta + C \left( \frac{1}{\lambda} - 1 \right) \right] C_1 + [\Delta + C(\lambda - 1)] C_2 = 0 \]  \hfill (32)

From Eqs. (28) - (32)

\[ u_1 = M_{Ng} \sigma_0 e^{-i\omega + iq \cdot \mathbf{x}} \]  \hfill (33)

where

\[ M_{Ng} = -\frac{\Delta (1 - \lambda^{2(N-1)}) - C(1 - \lambda)(1 + \lambda^{2N-3})}{\Delta^2(1 - \lambda^{2(N-1)}) - 2\Delta C(1 - \lambda)(1 + \lambda^{2N-3}) + C^2(1 - \lambda)^2(1 - \lambda^{2(N-2)})} \]  \hfill (34)

For \( N \to \infty \)

\[ \lim_{N \to \infty} M_{Ng} = -\frac{2}{\Delta + \sqrt{\Delta(\Delta - 4C)}} \]  \hfill (35)

For \(|\Delta/K| \ll 1 \) \( \gamma \to 1 \) thus the continuous medium approximation can be used for which the system (26) is reduced to equation

\[ \Delta u + a^2 C \frac{d^2 u}{dz^2} = 0 \]  \hfill (36)
FIG. 2: Dependence of the friction coefficient between water and graphene layers on number of graphene layers at $T = 300K$. Blue and brown points are for the van der Waals and electrostatic interaction at the potential difference $\varphi = 10V$. Blue and brown solid lines for the results obtained in the continuous medium approximation for the van der Waals and electrostatic interaction.

with the boundary conditions

$$\frac{du}{dz} \bigg|_{z=l} = 0, \quad aC \frac{du}{dz} \bigg|_{z=0} = -\sigma_0$$

where $l = Na$ is the thickness of the system of graphene layers. The solution of Eq. (36) has the form

$$u(z) = -\frac{\cos p(z - l)}{\sqrt{\Delta C \sin pl}} \sigma_0$$

(37)

where $p = \sqrt{\Delta/C}/a$. From (37)

$$M_{gl} = u(0)/\sigma_0 = -\frac{\cot pl}{\sqrt{\Delta C}}$$

(38)

For $l \to \infty$

$$\lim_{l \to \infty} M_{gl} = \frac{i}{\sqrt{\Delta C}}$$

(39)

IV. NUMERICAL RESULTS

The results of numerical calculations of the dependence of the friction coefficient $\gamma$ and heat transfer coefficient $\alpha$ between water and graphene system on the number of graphene layers $N$ are shown in Figs. 2 and 3. Blue (brown) points are for the system of $N$ discreet graphene layers and blue (brown) solid lines are obtained within the continuous medium approximation for the L.-J (electrostatic) interaction between surface displacements of water and graphene system. The $\gamma$ and $\alpha$ increase with $N$ for small $N$ and reach saturation for $N > 5$. At the saturation $\gamma_{LJ}^{sat} \sim 1500kg/m^2s$ and $\alpha_{LJ}^{sat} \sim 4 \cdot 10^7W/m^2K$ for the L.-J interaction. For the electrostatic interaction $\gamma$ and $\alpha$ reach maximum for the potential difference between water and surface graphene sheet $\varphi \sim 10V$ when at the saturation $\gamma_{el}^{sat} \sim 500kg/m^2s$ and $\alpha_{el}^{sat} \sim \alpha_{el}^{sat}$. For the water-graphene interface friction coefficient $\sim 10^5kg/m^2s$ was calculated using MD simulation. However, according to the experiments in Ref. $\gamma = 3 \cdot 10^3kg/m^2s$, which is only by factor 2 larger the value obtained in our calculations. Thus most likely MD simulation overestimate the water-graphene friction coefficient, which is typical in simulation of other water-solid system. The results for $\alpha_{LG}$ are in good agreement with the results obtained in Refs. 23,24 for the Kapitza resistance $R_K = 1/\alpha$ using MD simulations.
V. CONCLUSION

We have studied friction and heat transfer between water and a graphene system composed of graphene sheets. Unlike MD simulations, our theory does not require laborious numerical calculations. Numerical calculations of the dependence of the friction coefficient and heat transfer coefficient on the number of graphene sheets were performed. Our calculations of the friction coefficient are consistent with experimental data, but two orders of magnitude less than the values obtained using MD simulations. However, the results for the heat transfer coefficient are consistent with the results obtained using MD simulations. Radiative friction can be also important for water-carbon friction. For example, curvature dependence of friction observed for water in carbon nanotube can be explained by radiative friction produced by interlayer plasmons.\textsuperscript{32} However, the experiments in\textsuperscript{32} in large radius nanotubes can be explained by phononic friction. A strong enhancement in radiative friction is expected in the presence of an electric double layer on the water surface.\textsuperscript{33}

The reported study was funded by RFBR according to the research project N\textsuperscript{2} 19-02-00453

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