Finite-Size Effects in Nanoscale Lattice-Mismatched Lubricant Droplets

Relatore: Prof. Nicola Manini
Correlatore: Prof. Giuseppe Santoro

Andrea Nomellini
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Andrea Nomellini
Dipartimento di Fisica, Università degli Studi di Milano,
Via Celoria 16, 20133 Milano, Italia

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Abstract

In this work we study finite-size effects of nanoscale lubricant 2D droplets (or islands) by molecular dynamics. A small lubricant droplet is confined between two 2D crystalline layers; the bottom layer is static, while the top one slides rigidly. Simulations show that small nearly-lattice-matched islands can snap to commensuration entirely, changing their initial particle-particle distance $a_p$ to match the closest-in-registry lattice spacing $a_b$ so as to place epitaxially each lubricant particle in one energetically convenient hollow site of the bottom surface. For strongly mismatched islands instead, a solitonic pattern can remain trapped within the island, which deforms to a triangular-like shape. An overall droplet rotation during the snapping process is also observed under certain circumstance. Studying islands dragging phenomena, we find that commensurate snapped to commensuration droplets remain pinned to the bottom layer even when the top layer advances; while, when solitons are present and under favorable circumstances, the lubricant advances at some intermediate speed.

Advisor: Prof. Nicola Manini
Co-Advisor: Prof. Giuseppe Santoro
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Recent works [1, 2, 3, 4, 5] studied the lubricant friction problem for 2D infinite lubricant layers, and 1D finite-size chain [6, 7]. In the context of boundary lubricant, in this work we study finite size effects of nanoscale lubricant 2D droplets or islands by molecular dynamics. A lubricant island is represented by classic point-like Lennard-Jones (LJ) atoms, arranged in an approximately circular shape. The lubricant is sandwiched in between two substrates, represented by perfect 2D crystals. Each lubricant particle interacts with the other lubricant and substrate particles through a LJ potential. Lubricant particles are free to move in any direction, while the bottom layer is static and the top layer moves rigidly as a whole. We investigate how the snapping-to-commensuration phenomenon affects nearly-matched finite-size islands. Once we identify strongly mismatched islands which do not snap to commensuration and should therefore remain more mobile, we make the top layer slide, and verify under which conditions the lubricant droplets advances in between. While solitonic lines generally favor sliding, the presence of non parallel solitonic lines in mismatched islands can hinder lubricant dragging phenomenon.

Figure 1: The Lennard-Jones interaction energy, with $\varepsilon = 2$ and $\sigma = 1.7$. 

1 Introduction

Recent works [1, 2, 3, 4, 5] studied the lubricant friction problem for 2D infinite lubricant layers, and 1D finite-size chain [6, 7]. In the context of boundary lubricant, in this work we study finite size effects of nanoscale lubricant 2D droplets or islands by molecular dynamics. A lubricant island is represented by classic point-like Lennard-Jones (LJ) atoms, arranged in an approximately circular shape. The lubricant is sandwiched in between two substrates, represented by perfect 2D crystals. Each lubricant particle interacts with the other lubricant and substrate particles through a LJ potential. Lubricant particles are free to move in any direction, while the bottom layer is static and the top layer moves rigidly as a whole. We investigate how the snapping-to-commensuration phenomenon affects nearly-matched finite-size islands. Once we identify strongly mismatched islands which do not snap to commensuration and should therefore remain more mobile, we make the top layer slide, and verify under which conditions the lubricant droplets advances in between. While solitonic lines generally favor sliding, the presence of non parallel solitonic lines in mismatched islands can hinder lubricant dragging phenomenon.
2 The model

We represent the confining solid surfaces by two perfect crystalline 2D rigid layers, with hexagonal lattices representing, e.g. the (111) face of a cubic crystal. Between these rigid layers we insert a circular-shaped island of mobile lubricant atoms. Each atom composing the drop-like lubricant island is treated as a classical particle of unit mass \( m = 1 \). While the reciprocal positions of top and bottom substrate atoms are fixed, the atoms composing the lubricant island move freely under the action of pairwise LJ interactions between lubricant atoms themselves and between the lubricant atoms and the ones forming the top and the bottom layer. For the LJ interaction energy (see Fig. 1) we consider the expression

\[
\phi_{\text{LJ}}(r) = \varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - 2 \left( \frac{\sigma}{r} \right)^{6} \right], \tag{1}
\]

characterized by a minimum of depth \( \varepsilon \) at \( r = \sigma \). We truncate the interaction at a cut-off radius \( R_c = 2.5\sigma \) and shift the 2-body potential energy to eliminate the energy discontinuity as follows:

\[
\phi(r) = \begin{cases} 
\phi_{\text{LJ}}(r) - \phi_{\text{LJ}}(R_c) & r \leq R_c \\
0 & r > R_c 
\end{cases}. \tag{2}
\]

The motion of the \( j \)-th lubricant particle is ruled by the following equation:

\[
m \ddot{r}_j = -\sum_{i_t=1}^{N_t} \frac{\partial}{\partial r_j} \phi_{t,p}(|r_j - r^*_{i_t}|) + \\
- \sum_{j'=1, j' \neq j}^{N_p} \frac{\partial}{\partial r_j} \phi_{p,p}(|r_j - r^*_{j'}|) + \\
- \sum_{i_b=1}^{N_b} \frac{\partial}{\partial r_j} \phi_{b,p}(|r_j - r^*_{i_b}|) + \\
+ \vec{f}_{\text{damp},j} + \vec{f}_j(t), \tag{3}
\]

where \( r^*_j \) is the position of the \( j \)-th lubricant particle; \( r^*_{i_t} \) and \( r^*_{i_b} \) are the position of top and bottom atoms, \( N_t, N_p \) and \( N_b \) are the numbers of bottom, lubricant and top particles, and \( \phi_{b,p}, \phi_{p,p} \) and \( \phi_{t,p} \) are the truncated 2-body potential energies for the pair interaction between bottom-lubricant, lubricant-lubricant, and top-lubricant particles, respectively, characterized by specific \( \sigma \) and \( \varepsilon \) parameters. The gradient is computed as

\[
\frac{\partial}{\partial r_j} \phi(|r_j - r^*_{j'}|) = \frac{r_j - r^*_j}{|r_j - r^*_j|} \frac{\partial \phi(r)}{\partial r} \bigg|_{r = |r_j - r^*_j|}. \tag{4}
\]
By convention, we select the reference frame where the bottom layer is static. The top layer can be forced to move rigidly along \( x \) axis at a fixed horizontal velocity \( \dot{r}_{\text{top}}^{\text{ext}}(t) \equiv v_{\text{ext}} \). The top layer also moves rigidly along the \( y \) and \( z \) axis (its inertia equals the total mass of its atoms) under the interaction between the top itself and the lubricant layers. For these \( y \) and \( z \) components, the motion of \( i_t \)-th particle of the top layer is described by the following equations:

\[
N_t m_i \ddot{r}_{\text{top}}^{y(i)} = -\sum_{i'=1}^{N_t} \sum_{j=1}^{N_p} \frac{\partial}{\partial r_i^y} \phi^{t-p} (| r_i^y - r_j^z |),
\]

and

\[
N_t m_i \ddot{r}_{\text{top}}^{z(i)} = -\sum_{i'=1}^{N_t} \sum_{j=1}^{N_p} \frac{\partial}{\partial r_i^z} \phi^{t-p} (| r_i^y - r_j^z |),
\]

As all equations for \( r_{\text{top}}^{z(i)} \) and \( r_{\text{top}}^{y(i)} \) are the same, irrespective of \( i_t \), in practice their solution only differs for the initial arrangement \( \hat{r}_{\text{top}}^{\text{init}}(t) \equiv \hat{r}_{\text{top}}^{\text{ext}} + \hat{r}_{\text{init}}^{\text{init}} \). Here \( \hat{r}_{\text{init}}^{\text{init}} \) are the initial positions of the rigid top 2D lattice, and only the equations for \( \hat{r}_{\text{top}}^{\text{ext}} \) are integrated.

### 2.1 Friction work and thermostat

The total force needed to maintain the top layer motion at fixed velocity is given by the action-reaction principle: it equals the total force which the top exerts on the lubricant:

\[
F_{\text{frict}} = \sum_{i=1}^{N_t} \sum_{j=1}^{N_p} \frac{\partial}{\partial r_i^x} \phi^{t-p} (| r_i^x - r_j^x |),
\]

The work of this friction force

\[
W_{\text{frict}} = \int_0^\tau F_{\text{frict}} v_{\text{ext}} dt = \tau v_{\text{ext}} \bar{F}_{\text{frict}}
\]

represent the total Joule heat that the advancing top layer pumps into the mechanical system over an interval \( \tau \). To remove this Joule heat, reach a steady state, and control the lubricant temperature of this driven system, we use a standard implementation of the Langevin dynamics, derived by the damping term and the Gaussian random force \( \vec{f}_j(t) \) added to the deterministic force acting on each lubricant particle at the end of Eq. \([3]\). The damping force includes symmetric contributions representing the energy dissipation into both individual substrates

\[
\vec{f}_{\text{damp}j} = -\eta \dot{r}_j - \eta \left( \dot{r}_j - \dot{r}_{\text{top}} \right).
\]

Taking into account this twofold contribution to the \( \eta \)-dissipation, the null-average Gaussian random force satisfies the relation:

\[
\langle f_{jx}(t) f_{jx}(t') \rangle = 4 \eta k_B T \delta(t - t'),
\]
and similarly for the $y$ and $z$ components, such that in a non-sliding regime ($v_{\text{ext}} = 0$) the Langevin thermostat leads to a stationary state characterized by standard Boltzmann equilibrium average kinetic energy of the lubricant:

$$\langle E_k \rangle = \frac{3}{2} N_p k_B T. \quad (11)$$

This method represents a simple yet numerically stable and effective phenomenological approach to describe energy dissipation into the substrate occurring through the excitation of phonons and (in the case of metals) of electron-hole pairs. For lack of time, in the present work we will only simulate $T = 0$. To guarantee a detailed force balance (Newton’s third law), we add the following force term:

$$\eta \sum_i \left( \ddot{r}_i - \ddot{r}_t \right) = \eta N_p \left( \ddot{v}_{\text{cm}} - \ddot{r}_t \right) \quad (12)$$

to the equation for the motion of the top layer. While the $y$ and $z$ components of this additional term have a real influence on the motion of the top layer, the $x$ components only adds to the external force $F_{\text{frict}}$ [Eq. (7)] required to maintain the top velocity $x$ component constant and equal to $v_{\text{ext}}$. For faster island relaxation we adopt a large $\eta = 0.25$, while for dynamical simulations we use $\eta = 0.05$, leading to a highly under-damped regime.

### 2.2 Length scales and units

The system involves three generally different kinds of materials characterized by specific lattice spacings: $a_b$, $a_p$, $a_t$. We take LJ lengths $\sigma_{tt} = a_t$ and $\sigma_{bb} = a_b$. These LJ lengths are used only to determine $\sigma_{tp}$ and $\sigma_{bp}$ by means of the Lorentz-Berthelot mixing rules:

$$\sigma_{tp} = \frac{1}{2} (\sigma_{tt} + \sigma_{pp}), \quad \sigma_{bp} = \frac{1}{2} (\sigma_{bb} + \sigma_{pp}) \quad (13)$$

We take $\varepsilon_{bp} = \varepsilon_{tp} = \varepsilon$ for all pairwise coupling terms, while $\varepsilon_{pp}$ can assume different values. The relation between $\sigma_{pp}$ and $a_p$ will be discussed in Section 3.1.

We consider a set of “natural” units in terms of $\varepsilon$ (energy), $a_b$ (length), and $m$ (mass). All quantities are then expressed as dimensionless numbers, understanding that their value is referred to the natural units. To obtain a physical quantity in its explicit dimensional form, one should multiply its simulated numerical value by the corresponding natural units listed in Table I.

The spacing $a_b$, $a_p$, $a_t$ and the angles of relative rotation, define the initial conditions for the substrates and the lubricant island. Each layer is initially a
<table>
<thead>
<tr>
<th>Physical quantity</th>
<th>Natural units</th>
<th>Typical value</th>
</tr>
</thead>
<tbody>
<tr>
<td>length</td>
<td>$a_b$</td>
<td>0.2 nm</td>
</tr>
<tr>
<td>mass</td>
<td>$m$</td>
<td>50 a.m.u = $8.3 \cdot 10^{-26}$ Kg</td>
</tr>
<tr>
<td>energy</td>
<td>$\varepsilon$</td>
<td>1 eV = $1.6 \cdot 10^{-19}$ J</td>
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<tr>
<td>time</td>
<td>$a_b m^{1/2} \varepsilon^{-1/2}$</td>
<td>0.14 ps</td>
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<tr>
<td>velocity</td>
<td>$m^{-1/2} \varepsilon^{1/2}$</td>
<td>1400 m/s</td>
</tr>
<tr>
<td>force</td>
<td>$a_b^{-1} \varepsilon$</td>
<td>0.8 nN</td>
</tr>
</tbody>
</table>

Table 1: Natural units for several mechanical quantities in a system where length, mass and energy are measured in units of $a_b$, $m$, $\varepsilon = \varepsilon_{bp} = \varepsilon_{tp}$. Typical physical values are also reported.

perfect 2D hexagonal lattice, with the lubricant layer cut out in an approximately circular form.

The three different spacings $a_b$, $a_p$, $a_t$ give rise to two independent ratios affecting the lattice mismatches:

$$r_t = \frac{a_t}{a_p}, \quad r_b = \frac{a_b}{a_p}. \quad (14)$$

We perform the numerical integration of Eqs. (3), (5), (6) by means of an adaptive fourth-order Runge-Kutta-Fehlberg method.

2.3 Boundary conditions

To be able to explore many different configurations and to follow their evolution long enough, simulations must involve a number of atoms $N_p \simeq 10^3$, negligible compared to those involved in the realistic interface of macroscopic pieces of matters (easily of the order of $10^7$ in a $\mu$m²): such a large number of atoms would require massive computational resources. To alleviate this problem and impose precise lattice-spacing ratios, we use periodic boundary condition (PBC) in the $xy$ plane for the top and bottom layer: the particles are enclosed in a box generated by two vectors $\vec{a}_i^{\text{cell}}$ of length $L$. This supercell is replicated infinitely by means of rigid translations.

In the simple case in which the crystalline directions of the bottom and top lattices are parallel, it is straightforward to construct the appropriate supercell, which has the same alignment as the other lattices, and its side $L$ is taken as an integer multiple of both the top and bottom lattice spacing. The lubricant island, significantly smaller than $L$ in diameter, is not affected by the PBC, thus $a_p$ needs not be in any special relation to $L$. 
Figure 2: The average nearest-neighbor distance of an isolated finite size lubricant island at mechanical equilibrium as a function of the LJ minimum distance $\sigma_{pp}$. Initial particles distance $a_p = 1$, $\eta = 0.25$. In the calculation of $\langle d_{pp} \rangle$ for the $N = 2499$ island, only inner particles have been considered in order to avoid island-edge effects. Data are red, the green line represents the linear regression. An arrow indicates the intersection between linear regression and $\langle d_{pp} \rangle = 1$ line, at $\sigma_{pp} = \beta = 1.0083$.

3 Results

We come now to study the behavior of LJ finite-size droplets in the presence and even in the absence of confining perfect crystal layers. In particular we investigate the existence of the snapping-to-commensuration phenomenon and the droplets movement under the effect of a sliding top layer for different island sizes.

3.1 Relaxed island inter-particle spacing

The lubricant-bottom interaction is entirely ruled by pairwise couplings, which tend to favor the ”hollow” surface site compared to the ”bridge” and ”top” adsorption sites. The bottom-particle and particle-particle interaction defining parameters are $\varepsilon_{bp}$, $\varepsilon_{pp}$, $\sigma_{bp}$, $\sigma_{pp}$. While $\varepsilon_{bp} = 1$ and $\varepsilon_{pp}$ is arbitrary, $\sigma_{bp}$ is fixed ac-
According to the Lorentz-Berthelot mixing rules. As said above we assume $\sigma_{bb} = 1$, and we tune $\sigma_{pp}$. We should first relate $\sigma_{pp}$ to the droplet equilibrium geometry. In order to study snapping-to-commensuration phenomenon, we compare the lubricant particles spacing $a_p$ in ideal conditions, where no interaction with any other layer is present, to the situation when only the interaction with the bottom surface is present.

First of all, we want $a_p$ to represent the equilibrium particles distance of a non interacting relaxed lubricant island. The relaxed nearest-neighbor distance of an isolated island depends on the $\sigma_{pp}$ value. We study an isolated lubricant island with initial particle spacing $a_p = 1$, and determine its average nearest-neighbor particles distance $\langle d_{pp} \rangle$ at equilibrium as a function of $\sigma_{pp}$. This procedure allows us to evaluate the $\sigma_{pp}$ value (indicated by $\beta$) that makes the particles distance $a_p$ equal to unity.

We carry out simulations with different island size $N_p$. A quick $N_p = 102$ simulation allows us to locate the approximate relevant $\sigma_{pp}$-range. We then carry out a $N_p = 2499$ simulation. Figure 2 reports the resulting $\langle d_{pp} \rangle$ in the $N_p = 102$ and $N_p = 2499$ island simulations. In the larger island, inner particles interact very weakly with particles at the island edge. Because of that we will focus on $N_p = 2499$ island result as the most representative of the bulk case. By means of a linear fit of the $N_p = 2499$ nearest-neighbor distance, we evaluate the value $\beta$ of $\sigma_{pp}$ which produces a final equilibrium distance $\langle d_{pp} \rangle = 1$. The obtained data are compatible with $\beta = 1.0083$. This factor allows us to obtain a proportionality relation between $\sigma_{pp}$ and the nominal equilibrium spacing $a_p$, namely $\sigma_{pp} = a_p \cdot \beta$.

3.2 Snapping to commensuration

We come now to study the snapping to commensuration phenomenon. A deformable lubricant island interacts with a rigid-lattice mismatched crystal surface. The island is initially laid symmetrically around the supercell center in order to produce a round shape, with initial particle-particle distance $a_p$ and nominal mismatch ratio $r_b$. An example of initial and final relaxed configurations is shown in Fig. 3. The island and the bottom-layer crystal surface are initially parallel and aligned. Since the island does not reach across the periodic boundary conditions, and the island is small enough to remain inside the crystal supercell for all simulation time, it is allowed to undergo an overall relaxation, if energetically convenient. The system configuration is initially perfectly two-dimensional. Afterward island particles can relax along $z$ as well as in the lattice plane.

Simulations for $N_p = 102$ particles islands are carried on until the system reaches its mechanical equilibrium, namely when its total potential energy has
reached a local minimum. On this state we measure the final average spacing, and thus the resulting mismatch ratio $r'_b$. Island particles change their relative distance, at the same time maintaining an approximately bidimensional round shape. For nearly-matched values of $r_b$ the islands maintain almost perfectly their shape, while for under-matched and over-matched values of $r_b$ the overall shape changes a little due to a soliton pattern remaining trapped inside the island. An example is shown in Fig. 4. This island relaxes in a non-circular configuration where atoms are confined by a triangular pattern of solitonic lines.

The $r'_b$ dependency on $r_b$ in Fig. 5 shows the tendency to snapping to commensuration. For a nearly-matched island a nearly-flat plateau in $r'_b$ indicates that snapping has occurred. In the $N_p = 102$ island, this plateau in $r'_b$ extends over the $0.935 < r_b < 1.087$ region, for an intermediate-strength inter particle interaction $\varepsilon_{pp} = 1.0$. The plateau extends more in the over-dense $r_b > 1$ region than in the $r_b < 1$ region, because the $r_b < 1$ region is characterized by islands with $a_p > a_b$ which means that, to snap, lubricant particles should decrease their relative distance and match the bottom-layer lattice spacing. The LJ potential is highly repulsive below its minimum, see Fig. 1 thus decreasing lubricant particle distance is energetically more costly than increasing it. For lower values of $r_b$ we find no evidence of snapping to commensuration, although the system tends to decrease potential energy reducing the particle-particle distance slightly. Over-dense islands show several extra snapping to partial-commensuration plateaus. These far-from-commensuration islands snap to fractions of bottom lattice spac-

Figure 3: Unrelaxed initial (left) and relaxed (right) configuration of a $N_p = 999$ lubricant particles droplet (blue) on a perfect crystal surface (red). The initial mismatch ratio is $r_b = 1.064$. 
Figure 4: Initial (left) and relaxed (right) configuration of a \( N_p = 102 \) lubricant particles island, with rather large mismatched ratio \( r_b = 1.205 \). During the relaxation the island deforms and forms a triangular-shape solitonic line.

Figure 5: Final lubricant total energy (upper panel) and nearest-neighbor particle spacing (lower panel) for \( N_p = 102, \varepsilon_{pp} = 1.0 \) relaxed islands.
ing, showing a step-shaped curve trend. We observe partial-commensuration plateaus at height $r'_b \simeq 1.064, 1.087, 1.124$. We find no evidence of partial-snapping plateaus for $r_b > 1.205$, but we did not investigate the $r_b > 1.25$ region. The deeply overdense region is hard to explore because islands tend to abandon the epitaxial configuration and reconfigure in a three-dimensional bulky shape. The total relaxed energy reported in Fig. 5 shows that a snapped plateau tends to mark a local minimum of this energy, with the central region near commensuration gaining the most epitaxial energy, and paying smallest tribute to elastic deformation energy.

### 3.2.1 Dependence on self-binding-intensity

As we can expect, different values of the lubricant self-binding interaction energy $\varepsilon_{pp}$ lead to different results, reported in Fig. 6. The snapping to commensuration phenomenon is always observed, with the following differences. More rigid islands, $\varepsilon_{pp} = 1.5$, show a smoother $r'_b(r_b)$ dependence, with a more sloping central plateau that extends over a smaller interval, here $0.943 \leq r_b \leq 1.075$. Partial-snapping plateaus for overdense islands disappear, while the underdense region shows the same behavior as before. Softer islands, $\varepsilon_{pp} = 0.5$, exhibit a flatter snapping-to-
commensuration plateau at the nearly-matched region, extending over a broader interval, here $0.943 < r_b < 1.111$. The overdense region now displays a single broad partial-commensuration plateau, rather than several small plateaus. This plateau extends over the $1.124 < r_b < 1.205$ interval and it is centered around $r'_b = 1.087$. Even in the underdense region we now detect two small partial-commensuration plateaus, one in $0.917 < r_b < 0.926$ at mean spacing $r'_b \simeq 0.935$ and the other in $0.893 < r_b < 0.909$ at mean spacing $r'_b \simeq 0.909$.

3.2.2 Number of particles dependence

We come now to investigate the size dependence of the snapping-to-commensuration phenomenon, composing larger islands. In a island made of $N_p$ particles, $N_p \propto r^2$, where $r$ is the circular island radius, while the number of particles on the edge is $N_e \propto r$. So, for larger droplets, $f_e = \frac{N_e}{N_p}$ is smaller than for smaller ones. Edge particles have less neighbor particles to interact with, which means they are weakly bounded to the rest of the island than those near the center. Because of that we could expect a stronger and sharper snapping-to-commensuration evidence for bigger islands. In order to snap-to-commensuration, a large island needs to move the atoms far from island center further away from their initial
position than a small island. This forces large droplets to relax in configurations that represent local minimum of their potential energy. Such configurations are partially commensurate and usually contain solitonic patterns.

The epitaxial tendency of a larger island produces a flatter plateau in $r'(r_b)$. Figures 7 and 8 show the relaxed spacing for $N_p = 504$ and $N_p = 999$. The central plateau extends in $0.971 < r_b < 1.064$ interval for the $N_p = 504$ particle island and in the narrower $0.980 < r_b < 1.053$ interval for the bigger $N_p = 999$ island. In the over-dense region the $N_p = 504$ particles droplet shows a partial-commensuration plateau in $1.190 < r_b < 1.235$ range at $r'_b = 1.205$, together with several smaller partial-commensuration steps, producing a typical staircase. The $N_p = 999$ particles island shows a broad partial-commensuration plateau for $1.087 < r_b < 1.124$ at $r'_b = 1.053$. Both islands exhibit several small partial-commensuration steps in the under-matched region. Fig. 9 shows two partial-commensurate droplet configurations, characterized by a pattern of solitonic and
Figure 9: Relaxed configuration for a $N_p = 999$, $r_b = 1.111$ (left) and $r_b = 0.935$ (right) island. Three lubricant soliton (left) and anti-soliton (right) atoms occupy top sites, and several solitonic (left) and antisolitonic (right) lines are present.

Figure 10 combines the results for all three different $N_p$ and different $\varepsilon_{pp}$. Calculations show that the central commensurate plateau becomes flatter and shorter as the island size grows, and the partial-commensuration phenomenon become more well defined. Even though larger islands gain more energy in the snapping process, this process requires the displacement of more atoms when the island gets larger. Thus, underdense and overdense islands stabilize themselves by snapping to a partial commensuration, trapping solitons inside, when they are large enough. This is the reason why larger islands show shorter and stronger central snapping plateaus and multiple partial-snapping smaller steps. The $\varepsilon_{pp}$ dependence seems to play a small role in the snapping phenomenon than the size dependence, except for the smallest $N_p = 102$ particles island, where small $\varepsilon_{pp}$ favors a broader partial-snapping plateau in the over-dense region, of which there is no evidence in larger islands.

For comparison, we carry out simulations for $N = 999$ $\varepsilon_{pp} = 1$ islands for $r_b$ near the edge of the central snapping plateau ($0.943 < r_b < 0.971$ and $1.064 < r_b < 1.111$), with a different initial configuration. We prepare the initial island configuration with the lubricant particle-particle distance equal to $a_b = 1$, instead of $a_p$ as done before. The LJ particle-particle length is taken the same we used for previous simulations, $\sigma_{pp} = \beta a_b/r_b$. The initial lubricant spacing is now energetically favorable to the lubricant-bottom interaction, but energetically un-
Figure 10: Relaxed particles distance for different \( N_p \) and \( \varepsilon_{pp} \).
favorable to the lubricant inter-particle interaction. These simulations, see Fig. 8 (crosses and diamonds), lead to a wider central plateau in \( r_b' \), composed by lubricant relaxed configurations characterized by different mechanical lubricant energy than before. These new relaxed nearly-matched configurations are less energetically favorable in the overdense region near and outside the plateau’s edge, and more energetically favorable in all the underdense region and inside the plateau at the overdense side.

3.2.3 Rotations

Other works \[8, 9\] demonstrated the possibility of orientation transition in incommensurate structures and crystalline surface. Final configuration images indicate that certain islands rotate by a small angle \( \alpha \) around the \( z \) axis during relaxation. Even the pattern of Fig. ?? indicates a local tendency to rotations. Figure 11 shows a clean example of a global-rotation phenomenon. \( N_p = 102 \) particles islands exhibit the following rotation angles \( \alpha(r_b) \): \( \alpha(0.840) \simeq 3^\circ \), \( \alpha(0.847) \simeq -6^\circ \), \( \alpha(1.220) \simeq -7^\circ \), \( \alpha(1.235) \simeq 7^\circ \), \( \alpha(1.250) \simeq 7^\circ \). \( N_p = 504 \) particles islands settle on generally smaller rotation angles, e.g. \( \alpha(0.847) \simeq 0.5^\circ \), \( \alpha(0.855) \simeq 0.5^\circ \), \( \alpha(0.862) \simeq 3^\circ \). As far as our simulations can tell, even larger islands \( (N = 999) \), do not exhibit the spontaneous global rotation phenomenon. Instead for a number of islands the inner particles tend to rotate, while the outer ones remains stuck near their initial alignment. It would be instructive to explore the relax-
Figure 12: Movement of $N_p = 102$, $r_b = 1.149$ island under the effect of $a_t = 3.0$, $v_{ext} = 0.01$ sliding top layer (green). From left to right and up to down $t = 0$, $t = 1500$, $t = 3000$, $t = 4500$, $t = 6000$, $t = 7500$, frame is shown.

ation from initially rotated configurations, especially for large islands. However for lack of time this phenomenon is not investigated further.

### 3.3 Sliding top lattice

Several works [1, 2, 3, 4, 5, 6, 7] on sliding friction pointed out that a mismatched elastic layer confined between two crystalline surfaces can be dragged onto the bottom surface when the top surface moves under the effect of an external force. This is the standard behavior expected of a lubricant, but recent works [1, 2] found that under suitable conditions the lubricant layer moves at velocity $v_{cmx}$ such that its velocity ratio to the top speed $v_{ext}$ given by the following relation:

$$\omega = \frac{v_{cmx}}{v_{ext}} = \omega_{quant} = 1 - \frac{1}{r_b}.$$  \hfill (15)

For infinite layers, this phenomenon was interpreted as lubricant solitons created by the inertia with the bottom layer being dragged along by the moving top layer.
We call $a_{sol}$ the solitonic spacing. Solitonic lines represent in a certain way the excess (or lack) of lubricant particles with respect to the bottom particles. As one can easily verify, the solitonic spacing is related to the lubricant-atom spacing through:

$$a_{sol} = \frac{a_p}{a_p - a_b}.$$  \hspace{1cm} \text{(16)}

Introduced the $\theta = \frac{a_t}{a_{sol}}$ length ratio, it was shown that best results of sliding phenomenon are obtained when $\theta$ is unity, or at least a simple natural ratio of small integers [1, 2].

Here we investigate for the first time the sliding phenomenon for a finite lubricant island. This island does not need to satisfy the same supercell PBC as the top and bottom layers, and can therefore relax globally, as discussed in Sec. 3.2 above. Accordingly, for the $a_{sol}$ determination, in Eq. (16) for $a_p$ we do not use its initial nominal value, but rather the effective average spacing $a_b/r'_b$ determined by relaxation. As a result, no lubricant dragging is to be expected in the snapped plateaus.

We tested a number of islands with solitons. However, generally simulations done for $N_p = 102$ islands and $\theta = 1$ show no sliding phenomenon. Using $\theta = 0.5$ leads to the same results. The sliding phenomenon is not observed because $a_t = \theta a_{sol}$ is still comparable to the island radius. The top only perturbs the island crossing it, but is not dense enough to drag particles along.

Using a denser top layer, $a_t = 3.0$, with $v_{ext} = 0.01$ leads to different results. Snapped to commensurate islands still remain pinned to the bottom surface, while incommensurate islands are strongly perturbed by the top layer. Solitonic lines can follow the top layer movement if they are not parallel to $v_{ext}$. Parallel lines tend to remain pinned on the bottom surface. Accordingly, the island usually deforms, but eventually remains pinned to the bottom surface. Rotated islands are eventually rotated back to $\alpha = 0^\circ$ under the action of the sliding top layer. In the case $r_b = 1.149$ we find a peculiar reaction to the sliding top layer, illustrated in Fig. [12]. The upper half of the island advances, with the $60/120^\circ$ soliton lines following the top layer, while the lower half remains pinned to the bottom surface. This is because the upper half contains ready-to-move soliton lines and the lower half holds only a soliton line parallel to $v_{ext}$. After the detachment from the lower half, the upper half moves at velocity $\omega = 0.080$, close to $\omega_{quant} = 0.083$ obtained based on $r'_b$. Thus we find scarce but nonnull evidence of quantized velocity even for finite-size lubricant islands. Using even denser top layer, $a_t = 2.4$, and adding an external vertical load force $f_{load} = -0.1$ leads to very similar results. Few islands $r_b = 1.176, 1.190$ (upper half), 1.205 (upper half) initially move, but stop after a certain amount of time, when they run into a locked configuration. For
$a_t = 2.0$ and $f_{load} = -0.5$, the $r_b = 1.190$ island (upper half) initially moves, but stops after a while. This difficulty of dragging the $N_p = 102$ islands can be attribute to island edge particles, which are dominant for this small size. Edge particles are free to occupy energetically favorable sites and oppose to the movement of the solitonic lines, which are disposed non-parallel and too short to push efficiently forward the lubricant island.

We also carry out simulations for larger droplets, $N_p = 999$, for partial-commensurate relaxed configurations, $r_b = 0.885, 0.893, 0.901$. We adopt a top-layer spacing $a_t$ near to fraction of solitonic spacing $a_{sol}(r_b')$, namely values of $\theta = 1, 0.5, 4/3$. None of these configuration shows a lubricant-droplet movement.

4 Discussion and outlook

We find some preliminary evidence that under suitable conditions an island of finite size can realize the quantized sliding state. Furthermore systematic investigation is necessary to clarify the conditions for the presence/absence of the quantized sliding state.
References


