Relationship between contact size and static friction: An approach for rigid crystalline surfaces

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Abstract: Relationship between contact size (A) and static friction (f) has been studied for rigid crystalline systems. We built a series of systems with two identical surfaces but different orientations and investigated the effects of the size and shape of the contact area on static friction. In these systems, there are numerous nontrivial commensurate contacts. Our results confirmed that the relationship between A and f was determined by both commensurability and shape of the contact. For commensurate contacts, $f \propto A$ independent of the shape. For incommensurate contacts, generally $f \propto A^0$ for regular shapes or $f \propto A^{1/4}$ for irregular shapes; however, in very few cases of regular shapes, $f \propto A^{1/2}$. Moreover, in above systems, commensurability of a contact can be easily changed by a perturbation of the misfit angle. Therefore, if the perturbation caused by the lateral force and the deformation of the surface are considered (as is the case in real systems), further research is necessary.

Keywords: static friction; contact size; numeric simulation; rigid body

1 Introduction

Relationship between contact size and friction is one of the most essential and challenging issues in tribology. Classically, Amontons' law states that friction is independent of apparent contact size. Later, researchers have gradually realized that because of surface roughness, the actual contact area is a small proportion of the whole apparent contact area. This understanding is one of the foundations in modern tribology. Distinctly, friction only occurs in these small areas. Thus, friction is related to actual contact size and the relationship is generally considered to be linear.

Since 1980s, with the rapid development of nanotechnology, nanotribology has become an important branch of tribology [1–3]. In this new field, one crucial task is to understand the origin of the friction at the atomic level. To avoid being affected by other complex factors, a simple system with two clean and atomically flat crystalline surfaces is the most widely

studied model system. Theoretical studies first reported that, for an incommensurate and infinite contact, friction should be ultralow or even vanished in rigid systems or systems with weak coupling between surfaces [4, 5]. This prediction is supported by a series of experiments [6–9] and now is named as “superlubricity” or “structural lubricity” [10].

Structural lubricity corresponds to the case of $f \propto A^0$, where f is the static friction and A is the contact area. This is different from the usual linear relationship of $f \propto A$. In fact, they are the two most common cases of friction at the atomic scale. The structural lubricity state of $f \propto A^0$ has been achieved by many groups in different systems [9, 11–13], whereas $f \propto A$ is typically caused by the following two situations: one is obvious—both orientation and lattice parameters are exactly matched, and the other is that surface is poisoned by contaminants [14]. Furthermore, more complicated tribological behaviors have been observed in such a simple rigid system.

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For amorphous surfaces, Müser [15] predicted that $f \propto A^{1/2}$ and this prediction was supported by molecular dynamics simulations [16] and experiments [17]. For crystalline surfaces, de Wijn [18] studied the issue theoretically and focused on an application in heterogeneous surfaces: the sliding of gold nanoparticles on the surface of graphene, and five different relationships were predicted: $A^0, A^{1/2}, A^1$, when the shape of contact area was regular, and $A^{1/4}, A^{3/4}, A^1$, when the shape was irregular. These predictions were partially confirmed in experiments and simulations [17, 19].

In this study, we approached this issue in the systems with homogenous surfaces via numerical simulations. The interaction between two crystalline surfaces is described by Lennard-Jones (LJ) potential, which is more commonly used than the sinusoidal potential used in Refs. [18, 19]. Because energy dissipation can be neglected between two rigid surfaces, the origin of the static friction is the energy barrier that needs to be overcome in the sliding process. Thus, static friction f can be simply evaluated by the corrugation of the total potential energy ΔE_{tot} : $f \propto \Delta E_{\text{tot}}$ [17, 20]. We calculated potential energy surfaces (PES) for various rigid crystalline systems with two identical surfaces but different orientations (here “identical” means that two surfaces have the same lattice parameters). Our analyses also partially supported theoretical predictions by Ref. [18]. More specifically, for regular shapes, we observed all three predicted relationship between A and f : A^1 in commensurate contacts, A^0 in incommensurate contacts, and $A^{1/2}$ in very few cases. For irregular shapes, we only observed two of the three predicted relationships: A^1 in commensurate contacts and $A^{1/4}$ in incommensurate contacts. This phenomenon of friction depending on the shape of the contact area has also been commonly observed in recent studies [21–23]. However, we found some inconsistency with the literature. de Wijn [18] predicted a special type of commensurate contacts with $f \propto A^{1/2}$ for regular shapes and $f \propto A^{3/4}$ for irregular shapes, whereas we only observed very few instances for the former contact type.

Our results, together with those of previous studies [7, 9, 24] confirmed the importance of incommensurability for structural lubricity. But mathematically, there is no gap between commensurate and incommen-

surate contacts in two systems we studied here: a small change in the misfit angle can lead to the transition between commensurate and incommensurate contact. Therefore, as we discussed in this paper, the relationship between contact size and static friction in real systems is likely to be complex, necessitating further research.

2 Methods

2.1 Commensurate and incommensurate contacts

The terms “commensurability” and “incommensurability” are often mentioned when discussing structural lubricity and the opinion that structural lubricity is derived from incommensurate contacts is widely accepted. But most of the time when using these two terms, they were ambiguously synonymous with match or mismatch between two lattices, which led the commensurate contact to be often defaulted to the case that both orientation and lattice parameters were exactly the same. However, these terms can be precisely defined. From a geometric perspective, “commensurability” means that the geometric configuration of the contact area is periodically repeated in the two-dimensional (2D) plane (two examples are shown in Fig. 1). Consequently, besides the above trivial case, there are numerous nontrivial cases in commensurate contacts, which were first reported in square lattice by Gyalog and Thomas [25].

In this approach, we investigated static friction in rigid crystalline systems with two identical surfaces. As shown in Fig. 2, the two most common scenarios are considered: one is that both surfaces are $\langle 100 \rangle$ planes of the face centered cubic (FCC) lattice (Figs. 2(a)–2(c), refer to “square lattice” below), the other is that both surfaces are $\langle 0001 \rangle$ planes of the hexagonal close packed (HCP) lattice (Figs. 2(d) and 2(e), refer to “hexagonal lattice” below). For the former, as discussed in Ref. [25], a commensurate contact is obtained if the misfit angle θ satisfies the following conditions: both $\sin \theta$ and $\cos \theta$ are rational. Such qualified angles can establish a one-to-one correspondence to primitive Pythagorean triplets: for a Pythagorean triplet $a^2 + b^2 = c^2$, the bijective angle $\theta = \sin^{-1}(a/c)$ and the size of the smallest repeat unit is $\sqrt{c} \times \sqrt{c}$ (Fig. 1). We also termed such repeated 2D unit as “unit cell”,

Fig. 1 Commensurate contact between two identical crystalline surfaces. The lattices on two contact surfaces are shown in black dots (lower), red dots (upper) and blue dots (overlapped), respectively. (a) The trivial commensurate case in square lattice. In this case, the orientation is exactly the same ($\theta = 0^\circ$). The grey square area is the smallest repeat unit. (b, c) A nontrivial commensurate case in square/hexagonal lattice. The grey square area in the center is obviously repeated periodically (attention: the smallest repeat unit is the smaller grey square area shown in the upper left corner). The case of $(a, b, c) = (3, 4, 5)/(3, 5, 7)$ is shown here.

Fig. 2 Simulated systems. The top view of two contact surfaces is shown here. The lower surface is colored in red and the upper surface is colored in green. (a–c) Cases in square lattice (both surfaces are $\langle 100 \rangle$ planes of the FCC lattice), (d, e) cases in hexagonal lattice (both surfaces are $\langle 0001 \rangle$ planes of the HCP lattice). For each system, both surfaces contain three layers of atoms. The detailed size of the upper surface is listed in Table S2 (in the Electronic Supplementary Material (ESM)). The size of the lower surface is slightly larger to ensure that the minimum distance between two adjacent upper surfaces under periodic boundary conditions is greater than the cutoff distance 2.5σ .

although it is slightly different from the “unit cell” in crystallography—Its lattice points span two surfaces. For the latter, according to the requirement of periodic repetition, it is easy to know that there is a one-to-one correspondence between misfit angles θ of commensurate contacts and primitive solutions of the following Diophantine equations: $a^2 + ab + b^2 = c^2$. The bijective function is $\theta = \sin^{-1}(\sqrt{3}a/2c)$ and the unit cell size is also $\sqrt{c} \times \sqrt{c}$ (Fig. 1). For both scenarios, all commensurate contacts with $c \leq 400$ are listed in Table S1 (in ESM). In addition, for convenience, in the following sections whether a contact is commensurate or not is simply determined by its misfit angle, although the size of the contact area may be smaller than the size of the unit cell and the periodic repetition in contact area does not actually occur.

Furthermore, it should be noted that in above two scenarios not only the number of commensurate contacts is infinite, but also any incommensurate contact can be approximated with arbitrary precision by a commensurate contact. A brief illustration for this assertion in square lattice is given here. Pythagorean triples $a^2 + b^2 = c^2$ can be generated by Euclid's formula: $a = m^2 - n^2, b = 2mn, c = m^2 + n^2$ (m and n are integers). Obviously, for any θ , $\sqrt{(1 + \sin \theta)/(1 - \sin \theta)}$ can be approximated by rational number m/n , which is equivalent to that any $\sin \theta$ can be approximated by $a/c = (m^2 - n^2)/(m^2 + n^2)$.

2.2 Calculation of potential energy surface

We investigated PESs of various rigid crystalline systems. In these systems, interactions between two surfaces were calculated by LJ potentials, which had been widely used to simulate various atomic scale systems including friction, wear, and lubrication [26, 27]. As one of the most popular pairwise potentials, LJ potential is a good approximation of the interaction between neutral atoms or molecules and the formula.

$$E_{\text{LJ}}(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (1)$$

where r is the distance between two particles, ε and σ represent the length and energy scale, respectively, varied for different substances. Obviously, the

interaction strength between two neutral particles decays very rapidly with the increase of r . Thus, LJ potential is often truncated at a cut-off distance of $r_c = 2.5\sigma$ as follows:

$$E_{\text{LJ}_{\text{trunc}}}(r) = \begin{cases} E_{\text{LJ}}(r) - E_{\text{LJ}}(r_c) & (r \leq r_c) \\ 0 & (r > r_c) \end{cases} \quad (2)$$

In this study, firstly we examined commensurate systems with only a single unit cell. As mentioned earlier, the size of the unit cell is limited to $c \leq 400$. Totally, there are 64 cases for square lattice and 54 cases for hexagon lattice (the trivial case with misfit angle $\theta = 0^\circ$ is included). For each case, we constructed a system with three layers of atoms on each of the upper and lower surfaces, and periodic boundary conditions were applied. Both two surfaces were flat, atomic smooth, and placed in parallel with a fixed distance. Both surfaces were treated as rigid bodies and a truncated LJ potential with the cut-off distance of $r_c = 2.5\sigma$ was used to describe their interactions. The total average interaction force between surfaces was zero, which meant that the load was zero. The particular distance was obtained by enumeration. Moreover, because we were concerned with the relationship between the static friction force f and the contact size A , not the actual value of f , all calculations were performed with dimensionless (or reduced) unit (both ε and σ were set to 1). Then the PES of the system was obtained by sampling. When sampling, lower surface was fixed and only the upper surface was moved. Due to the periodicity of the crystalline surface, the sliding range was within a single unit cell of the lower surface. The sampling was carried out in a 200×200 grid and all calculations were performed by large-scale atomic/molecular massively parallel simulator (LAMMPS) [28].

Next, systems with contact areas of various sizes and shapes were examined. We changed the size and shape of the upper surface and always kept the lower surface large enough. Because two surfaces are still flat and atomic smooth, the size of the contact area can be simply presented by the number of atoms in the lowest layer of the upper surface. Specifically, as shown in Fig. 2, for square lattice, we considered three shapes—square, rectangle, and circle, and for

hexagonal lattice, we considered two shapes—rectangle and circle. In these systems, both surfaces have three layers of atoms and the size of the contact area is listed in Table S2 (in ESM). PESs for different misfit angle θ were calculated in the same manner. These angles were divided into two groups. One group corresponded to commensurate contacts and all cases with $c \leq 400$ were calculated (16 cases in square lattice and 14 cases in hexagonal lattice, the trivial case with misfit angle $\theta = 0^\circ$ is excluded). The other group corresponded to incommensurate contacts and the misfit angle was scanned in step of 1° . Due to the symmetry of the lattice, totally there were 45 cases in square lattice (from 1° to 45°) and 30 cases in hexagonal lattice (from 1° to 30°).

3 Results and discussion

3.1 f is always linearly correlated to A in commensurate contacts

For commensurate contacts, we first calculated PESs of a single unit cell. Double logarithmic plots between the corrugation of the potential energy $\Delta E_{\text{unit}}(\theta)$ (which was a per-atom value) and the number of atoms M in the single unit cell are shown in Fig. 3. These graphs

Fig. 3 $\Delta E_{\text{unit}}(\theta)$ versus M of commensurate systems with a single unit cell. $\Delta E_{\text{unit}}(\theta)$ is the corrugation of per-atom potential energy and M is number of atoms in contact area. Various sizes of commensurate systems with a single unit cell (the details are listed in Table S1 in the ESM) are calculated. Evidently, there is a linear relationship in double logarithmic plots, which means $\Delta E_{\text{unit}}(\theta) \propto M^C$.

clearly indicate a power law correlation $\Delta E_{\text{unit}}(\theta) \propto M^C$ in both square and hexagonal lattices, and the exponent C is approximately $-4/3$ for large values of M . In addition, we found that f was much smaller in all nontrivial commensurate contacts than in the trivial commensurate contact ($\theta = 0^\circ$), which may be the reason why such commensurate contacts were not noticed in the previous experiment [9].

Next, the effects of size and shape of the contact area were considered. As described in Section 2, three shapes were inspected in square lattice: two were regular (square and rectangle) and one was irregular (circle). The number of atoms in the contact area ranged from several hundred atoms to $\sim 250,000$ (details in Table S2 (in ESM)). For each commensurate contact with misfit angle θ , we calculated $\Delta E(\theta, A, S)$ for all size A and shape S , and compared them with $\Delta E_{\text{unit}}(\theta)$. Representative cases are shown in Fig. 4. Evidently, when A or N increases, $\Delta E(\theta, A, S)$ converges to $\Delta E_{\text{unit}}(\theta)$ and in the case of regular shapes, the convergence is much faster (as shown in Figs. 4(a)–4(c)). In addition, the rate of convergence also depends on the size of the unit cell c and misfit angle θ . The effect of c is shown in Figs. 4(d) and 4(e). Clearly, a larger c results in a slower rate of convergence and the rate seems to be inversely proportional to c (see Fig. 4(e)). The effect of θ is shown in Fig. 4(f): a smaller θ ($\theta \leq 10^\circ$) leads to a slower rate. Similar results were obtained for the hexagonal lattice (Fig. S1 in ESM). We note $\Delta E(\theta, A, S)$ is a per-atom value and $\Delta E_{\text{unit}}(\theta)$ is a constant independent of A . These results demonstrate that f is always linearly correlated to A in commensurate contacts ($f \propto N \Delta E(\theta, A, S) \propto A \Delta E_{\text{unit}}(\theta) \propto A$) regardless of the shape of the contact area.

The geometric configuration of the contact area can help us better understand the above results. The PES between two crystalline surfaces can be regarded as the superposition of a series of PESs between one atom and the crystalline surface. Because the crystalline surface is periodic, the PESs involved in the superposition are the same functions but with different phases. Here phase is 2D and can be represented as a point on a 2D plane straight forwardly. In commensurate contacts, the number of different phases is finite and equal to c . One example is given in Fig. 5(a). For the commensurate contact in the square lattice corresponding to a

Fig. 4 $\Delta E(\theta, A, S)$ of commensurate systems with FCC lattice. r is ratio of $\Delta E(\theta, A, S)$ to $\Delta E_{\text{unit}}(\theta)$, N is number of atoms in contact area, and $M = N/c$ is number of minimum repeat units in contact area. (a–c) show the effects of shape and size of the contact area, (d, e) show the effect of the size c of the unit cell, and (f) shows the effect of misfit angle θ . Obviously, when N becomes larger, r gradually converges to 1 in all cases. Moreover, for irregular shapes, large c and smaller θ ($\theta \leq 10^\circ$) lead to slower rate of convergence. The rate is inversely proportional to c and is more sensitive to shape and θ .

Fig. 5 Geometric configuration of the contact surfaces. The PES between two crystalline surfaces $E = F(x, y)$ is a superposition of a series of PESs between one atom and the crystalline surface $E = \sum E_i = \sum f_i(x, y)$. Due to the periodicity of the crystalline surface, these superposed PESs are the same functions but with difference phases ($f_i(x, y) = f(x + \Delta x_i, y + \Delta y_i)$) and we term $(\Delta x_i, \Delta y_i)$ as the phase for atom i). One example is shown in (a), which is a commensurate contact with misfit angle $\theta = \sin^{-1}(3/5) = 36.87^\circ$ and size $A = c \times c = 5 \times 5$ (in reduced unit). The left side of (a) is the top view of the contact surfaces and the atoms are colored by black (lower), red (upper), and blue (overlapped), respectively. The right side of (a) shows the distribution of the phases. There are only $c = 5$ different phases (shown in red dots) and they can correspond to c adjacent atoms on a straight line. (b) shows an incommensurate contact with $\theta = 45^\circ$ in the same manner. Evidently, the phases are distributed on a series of lines parallel to the X axis. (c) shows phase distributions of two incommensurate contact with the same misfit angle, similar size but different shapes. Here $\theta = 28^\circ$ is very closed to $\theta = \sin^{-1}(8/17) = 28.07^\circ$, which is a commensurate contact with $c = 17$. Therefore, the points in the phase space are distributed into 17 clusters when the size is not too large. But for points in each cluster, the distribution is square when the shape of the contact area is square, and fan-shaped when the shape of the contact area is circle. Obviously, the latter is more biased.

Pythagorean triple $(a, b, c) = (3, 4, 5)$, there are only $c=5$ different phases. Thus, for a contact with any size and shape, the final PES is always a weighted combination of c basic PESs. Moreover, the simplest geometric configuration of atoms corresponding to a set of the c basic PESs, is where c atoms are placed side by side in a straight line — $1 \times c$ or $c \times 1$ (Fig. 5(a)). For any shape, it can be split into combinations of $1 \times c$ and $c \times 1$ with some extra scattered parts. If the feature size of the shape is R , the area of the scattered parts is on the order of R , but the total area is on the order of R^2 . Thus, when R tends to infinity, the effect of these scattered parts can be ignored, resulting in a shape-independent relationship between f and A .

3.2 Relationship between f and A depends on the shape of the contact area in incommensurate contacts

The same systems as above but with different misfit angle θ were examined. The effect of θ was systematically investigated by scanning. Then PESs and corrugations $\Delta E(\theta, A, S)$ were calculated for these incommensurate systems and the results were

shown in Figs. 6 (square lattice) and S2 in the ESM (hexagonal lattice).

As shown in Figs. 6(a)–6(c), in most cases of square lattice, there is also a good power law correlation between $\Delta E(\theta, A, S)$ and A : $\Delta E(\theta, A, S) \propto N^C \propto A^C$. But for different types of shapes, the value of the exponent C is different: $C \approx -1$ for regular shapes and $C \approx -3/4$ for irregular shapes (Fig. 6(d)). Equivalently, this means that for commensurate contacts, we have $f \propto A^0$ for regular shapes or $f \propto A^{1/4}$ for irregular shapes. Similar results were obtained for hexagonal lattice (Fig. S2 in ESM). These results reveal that the relationship between f and A depends on the shape of the contact area and reconfirm the predictions in Ref. [18].

It is also helpful to examine the geometric configuration of the contact area for understanding these results. In an incommensurate contact, the phase of the superimposed PESs is always different with each other. Two examples with the same θ but different shapes are shown in Fig. 5(c). Because the angle $\theta = 28^\circ$ is very closed to the angle of a commensurate contact $\theta = \sin^{-1}(8/17) = 28.072^\circ$, the phase dots are grouped into 17 clusters in both shapes when the size A is not

Fig. 6 $\Delta E(\theta, A, S)$ of incommensurate systems with FCC lattice. (a–c) are double logarithmic plots between $\Delta E(\theta, A, S)$ and N with different misfit angles and shapes. Clearly, there are $\Delta E(\theta, A, S) \propto N^C$ in all cases. (d) shows the distribution of the exponent C . In most cases, C is around -1 for regular shapes (square and rectangle) and C is around -0.75 for irregular shapes (circle). In very few cases of regular shapes, C is around -0.5 . (e) shows double logarithmic plots between $\Delta E(\theta, A, S)$ and N in three specific cases ($\theta = 30^\circ/45^\circ$ in FCC lattice and $\theta = 30^\circ$ in HCP lattice) with $C \approx -1/2$. (f) shows the distribution of the exponent C when any one of $\sin\theta$, $\cos\theta$, and $\tan\theta$ is rational. Clearly, the expected cases of $C = -1/2$ for regular shapes or $C = -1/4$ for irregular shapes do not occur.

too large. The difference between the two cases is: For the regular shape (square), the distribution of points within each cluster is symmetric and unbiased, but for the irregular shape (circle), the distribution is fan-shaped and biased. Consequently, when A tends to infinity, the distribution of all points is also symmetric and unbiased for the former but asymmetric and biased for the latter. So, the corrugations of superimposed PESs are largely cancel each other in an unbiased distribution, which gives rise to $f \propto A^0$ for regular shapes, and the corrugations of superimposed PESs are still residual in a biased distribution, which give rise to $f \propto A^{1/4}$ for irregular shapes.

3.3 $f \propto A^{1/2}$ for some very specific cases

Although in most cases f and A follow the relationship of $f \propto A^0$ or $f \propto A^{1/4}$, very few cases are exceptional. We noticed the following three cases: regular shapes with $\theta = 30^\circ$ or $\theta = 45^\circ$ in square lattice, and regular shape with $\theta = 30^\circ$ in hexagonal lattice. In these cases, there are significant oscillations in the double logarithmic plot of $\Delta E(\theta, A, S)$ and N (Fig. 6(e)), which result in a low coefficient of determination ($R^2 \approx 0.5$). But power law correlations $-\Delta E(\theta, A, S) \propto N^C$ are still observed and the value of the exponent C is around -0.5 , which means $f \propto A^{1/2}$.

In the same manner, we examine the geometric configuration of the contact area again and find that in these cases the phase distribution is also biased: corresponding points in two-dimensional plane are distributed on lines parallel to the primitive vectors (Fig. 5(b)). In square lattice, this bias is occurred when any one of $\sin\theta$, $\cos\theta$, and $\tan\theta$ is rational and the case of $\theta = 30^\circ$ and $\theta = 45^\circ$ meet this requirement. A brief explanation is given here. For two grid points (x_1, y_1) and (x_2, y_2) , after rotating θ clockwise, the new coordinates are $(x'_1, y'_1) = (x_1 \cos\theta - y_1 \sin\theta, x_1 \sin\theta + y_1 \cos\theta)$ and $(x'_2, y'_2) = (x_2 \cos\theta - y_2 \sin\theta, x_2 \sin\theta + y_2 \cos\theta)$. When $(y'_2 - y'_1)$ is an integer, the corresponding points in the phase space have the same ordinate, which means that they are distributed on a straight line parallel to the x axis. Obviously, $(y'_2 - y'_1)$ is an integer requires that any one of $\sin\theta$, $\cos\theta$, and $\tan\theta$ is rational. de Wijn [18] also predicted a special type of commensurate contacts with $f \propto A^{1/2}$ in regular shapes

and $f \propto A^{3/4}$ in irregular shapes. The requirement of these “commensurate contacts” for square lattice given in Ref. [18] is that only one of $\sin\theta$ and $\cos\theta$ is rational, which is very similar to our above requirements. We investigated more cases with θ to satisfy these requirements. However, the relationship of $f \propto A^{1/2}$ has never appeared again and the relationship of $f \propto A^{3/4}$ has never been found (Fig. 6(f) for the distribution of the exponent C in these cases).

3.4 Relationship between f and A in actual cases

Above results imply that whether a contact is commensurate or not is crucial for static friction f . However, on the one hand, just as the probability that a real number is rational is zero, the probability that a contact is commensurate is also zero. On the other hand, as mentioned earlier, if only considering misfit angle θ , commensurate contact can approximate any incommensurate contact with arbitrary precision. Therefore, the property of the function $f = f(\theta, A, S)$ is very poor mathematically: when A tends to infinity, f is discontinuous everywhere for θ . Moreover, our simulated systems are highly idealized: both two surfaces are rigid bodies and the misfit angle θ is always fixed. But for actual cases, the deformation of the surface and the perturbation of the misfit angle θ caused by the lateral force should be considered. Thus, an interesting question is: What is the real relationship between contact size A and static friction f ?

Here we provide some insights into this question. First, after a perturbation on misfit angle θ , the change of static friction f was examined for commensurate contacts. Then we made comparisons and two typical cases in square lattice were shown in Fig. 7. One is the comparison between $\theta = \sin^{-1}(3/5) = 36.870^\circ$ (commensurate) and $\theta = 37^\circ$ (incommensurate). In this case, for the incommensurate contact, there is a plateau on the curve for small size, which is caused by its adjacent commensurate contact indeed. The other is the comparison between $\theta = \sin^{-1}(39/89) = 25.989^\circ$ (commensurate) and $\theta = 26^\circ$ (incommensurate) for which the plateau does not exist. Certainly, although the difference of θ is very small in both cases, there is a large variance in $\Delta E(\theta, A, S)$ when N is large, which reconfirms the discontinuity of the function $f = f(\theta, A, S)$.

Fig. 7 Comparisons between commensurate contact and incommensurate contact with small difference in θ . $\Delta E_{\text{unit}}(\theta)$ versus N is shown for commensurate contact and $\Delta E(\theta, A, S)$ versus N is shown for incommensurate contact. (a) is the comparison between $\theta = \sin^{-1}(3/5) = 36.870^\circ$ (commensurate) and $\theta = 37^\circ$ (incommensurate). (b) is the comparison between $\theta = \sin^{-1}(39/89) = 25.989^\circ$ (commensurate) and $\theta = 26^\circ$ (incommensurate). When N is small, only in the case of A , there is a plateau of $\Delta E(\theta, A, S)$ in incommensurate contacts and the plateau is closed to $\Delta E_{\text{unit}}(\theta)$ of the commensurate contact. When N is large enough, in both cases there is a significant difference in $\Delta E(\theta, A, S)$ between commensurate and incommensurate contact.

These observations suggest that: For a commensurate contact, when size is small, a perturbation on θ may not cause a sharp drop in static friction f and the system may still remain in the state of high friction; by contrast when size is large, such perturbations will always lead to the system into the state of structural lubricity. However, if considering the potential energy of different contacts, the case will be different. Filippov et al. [29] reported that the system was locked to the trivial commensurate state with high friction by rotations. To avoid the destruction of the structural lubricity, some suggestions were given in Ref. [30] and were partially supported by experiments in Ref. [31]. We also find that for a given size and shape, the average of their PESs is equal for different θ . So, the greater the corrugation, the smaller the minimum value on the PES. Thus, if there is a slight perturbation on θ during the sliding process, the system would easily be trapped to these minimal cases of the nontrivial commensurate contacts and exit to the state of structural lubricity. These contradictory results indicate that the relationship between f and A is highly complicated even without the consideration of the deformation.

4 Conclusions

In this study, we investigated the relationship between contact size and static friction systematically in rigid

crystalline systems with two identical surfaces. Geometrically, according to the misfit angle θ , there are two types of contact: Commensurate and incommensurate. In the former the geometric configuration of the contact area is periodically repeated, while in the latter it is not. We constructed a series of systems with contact areas of various sizes and shapes and examined their PESs. Our results indicate: 1) when contact is commensurate, $f \propto A$, 2) when contact is incommensurate, depending on the shape of the contact area, the relationship can be $f \propto A^0$ (regular shapes) or $f \propto A^{1/4}$ (irregular shapes), 3) for very rare cases, $f \propto A^{1/2}$.

These results reconfirm the importance of commensurability. They also implies that: For a particular shape S , when A tends to infinity, f is discontinuous everywhere for θ . This conclusion is confirmed by our numerical simulations: when A is large, a perturbation on θ always causes a significant drop in f . It seems that if A is sufficiently large, structural lubricity can always be achieved. However, from an energetic perspective, the system can reach a lower energy state for a commensurate contact; thus, the incommensurate system tends to be locked to the contiguous commensurate contact. Moreover, in real systems the deformation should be considered. Therefore, further research is deserved for this issue.

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