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Nano-friction phenomenon of Frenkel–Kontorova model under Gaussian colored noise

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The nano-friction phenomenon in a one-dimensional Frenkel–Kontorova (FK) model under Gaussian colored noise is investigated by using the molecular dynamic simulation method. The role of colored noise is analyzed through the inclusion of a stochastic force via a Langevin molecular dynamics method. Via the stochastic Runge–Kutta algorithm, the relationship between different parameter values of the Gaussian colored noise (the noise intensity and the correlation time) and the nano-friction phenomena such as hysteresis, the maximum static friction force is separately studied here. Similar results are obtained from the two geometrically opposed ideal cases: incommensurate and commensurate interfaces. It was found that the noise strongly influences the hysteresis and maximum static friction force and with an appropriate external driving force, the introduction of noise can accelerate the motion of the system, making the atoms escape from the substrate potential well more easily. Interestingly, suitable correlation time and noise intensity give rise to super-lubricity. It is noteworthy that the difference between the two circumstances lies in the fact that the effect of the noise is much stronger on triggering the motion of the FK model for the commensurate interface than that for the incommensurate interface.

Keywords: Frenkel–Kontorova model, Gaussian colored noise, hysteresis, super-lubricity

PACS: 05.10.Gg, 68.35.Af, 81.40.Pq, 83.10.Rs **DOI:** 10.1088/1674-1056/ac439d

1. Introduction

Nano-friction is becoming more and more often a central issue in the emerging field of nanoscale science and technology, which is related to the atom processes occurring at the interface of two interacting systems in relative motion.[1–3] Recently, remarkable achievements have been made in nano-friction testing technology (atomic and friction force microscope, surface-force, and quartz-crystal microbalance) and the computing power (realistic molecular dynamics simulations). And these advances have largely encouraged to search for simple mathematical models capable of describing the essential physics in friction processes.[3] In particular, the driven Frenkel–Kontorova (FK)[4] models have recently received an increasing amount of attention and have been extensively investigated both theoretically and experimentally in the nano-friction areas.[5,6] The standard FK[3,4] model describes the dissipative motion of a chain of harmonically interacting particles that slides over a rigid substrate potential due to the application of an external driving force. Moreover, the classic FK model has been used to study the dynamic phenomena in nano-tribology, and an increasing interest as a possible interpretative key has been found to understand the atomic processes occurring at the interface of two materials in relative motion.[1–21] So far, the FK models have become an extremely important theoretical tool in the field of nano-tribology. Relevant generalizations of the FK models have also been proposed in the literature to cover a large class of physically interesting nano-friction phenomena,[7–13] such as hysteresis, super-lubricity, and stick-slip, *etc*. Furthermore, both the dynamics process of friction and the mechanism of energy dissipation on the nanoscale are explained, according to the FK models and nano-friction.

However, most studies on FK models focus on deterministic systems,[7–13] and only a few involves the stochastic systems.[15–20] In fact, noise is usually inevitable as modeling a real system at the nanoscale level. Tekić *et al.*[15–18] studied the noise effects on the dynamical mode-locking phenomena in the overdamped FK model. The effects of the temperature and substrate disorder on the FK model are investigated by Guerra *et al.*[19] The noise,[20,22] as a stochastic excitation, can not only make deterministic systems random but also change their dynamical behaviors. The interference of random factors is an important factor that cannot be ignored in the study of nonlinear dynamics. The random factor refers to Gaussian white noise or some associated colored noise. As the spectrum of Gaussian white noise[20] is unbounded and there is no Gaussian white noise in nature, the introduction of Gaussian white noise may go against the essential characteristics of some systems in nature. So the introduction of colored noise is very necessary. Therefore, the study of stochastic FK models under colored noise excitation has important practical significance for the understanding of nano-friction mechanism. This paper mainly studies the FK model under the Gaussian colored noise excitation and studies the variation of some nano-friction

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phenomena, such as hysteresis, maximum static friction force, and super-lubricity. The Langevin molecular dynamics approach allows us to introduce Gaussian colored noise via the inclusion of a stochastic force.[19,20] Working in the dissipative regime, we analyze the display of hysteretic behavior in the $B(F)$ characteristics[19] for the variation of the external driving force and the relationship between the maximum static friction force and the noise parameters.

The rest of the paper is organized as follows. Section 2 introduces the driven FK model with the Gaussian colored noise excitation. In Section 3, the simulation results are presented. The effects of different parameters (such as the noise intensity and the correlation time) on the chain mobility and the maximum static friction force have been investigated in detail for incommensurate case and commensurate case, respectively. Finally, the main conclusions are drawn in Section 4.

2. Model

The system here describes the dynamics of a driven FK model, whose N particle positions x_i satisfy the following equation of motion:[3,19,20]

$$m\ddot{x}_i + m\gamma\dot{x}_i + \frac{1}{2}\left(\sin\frac{2\pi}{a}x_i + \sin\frac{2\pi\beta}{a}x_i\right) + \frac{\mathrm{d}}{\mathrm{d}x_i}\left[\sum_{i\neq j} V_{\mathrm{int}}(|x_i - x_j|)\right] = F + \eta(t), \tag{1}$$

where m is the mass of particle. The dots denote time derivatives and γ is the damping coefficient. The geometry of the substrate potential is defined via the values of the two spatial periodicities a and $c = a/\beta$. The numerical simulations are carried out by choosing a Morse-type potential[2,14]

$$V_{\mathrm{int}}(r) = \frac{K}{2}[1 - \mathrm{e}^{(b-r)}]^2, \tag{2}$$

with the strength K and natural equilibrium spacing $b = L/N$, where L is the chain length. In order to avoid effects due to the boundary layers, the periodic boundary conditions

$$x_{i+N} = x_i + Nb. \tag{3}$$

In Eq. (1) F represents the external driving force applied to all atoms of the chain. The last term $\eta(t)$ is the exponentially correlated, Gaussian colored noise with zero mean.[22] The correlation properties of $\eta(t)$ can be written as

$$\begin{cases} \langle \eta(t) \rangle = 0, \\ \langle \eta(t)\eta(s) \rangle = D\lambda \exp(-\lambda|t-s|), \end{cases} \tag{4}$$

where D is the noise intensity and the correlation time $\tau = \lambda^{-1}$.

Equation (1) with properties (4) can be replaced with the white-noise equations

$$\begin{cases} m\ddot{x}_i + m\gamma\dot{x}_i + \frac{1}{2}\left[\sin\frac{2\pi}{a}x_i + \sin\frac{2\pi\beta}{a}x_i\right] \\ + \frac{\mathrm{d}}{\mathrm{d}x_i}\left[\sum_{i\neq j} V(|x_i - x_j|)\right] = F + \eta(t), \\ \dot{\eta}(t) = -\lambda\eta(t) + \lambda\xi(t). \end{cases} \tag{5}$$

The initial η_0 distribution is given by

$$P(\eta_0) = \frac{1}{(2\pi D\lambda)^{1/2}} \exp\left[-\frac{\eta_0^2}{2D\lambda}\right]. \tag{6}$$

To deal with the random terms in Eq. (5), a stochastic extension of the standard Runge–Kutta algorithm[22] is implemented for the colored-noise equations. The system is initialized with the particles placed at rest at the uniform separation b. The chain is driven by the external force F, which is increased or decreased. For every value of F and after reaching the dynamical steady state, the system characteristics of relevant physical interest are measured. The final chain configuration (positions and velocities) obtained at one value of F is used as the initial condition for the next value of the driving. The center of the mass (CM) average velocity of the chain is defined as

$$V_{\mathrm{CM}} = \frac{1}{NT}\int_0^T v_i. \tag{7}$$

The ratio $B = V_{\mathrm{CM}}/F$ of the time-averaged CM velocity to the external applied force (the chain mobility).[19] Observation of finite static friction implies that the contacting solids have locked into a local energy minimum, and F_{s} is maximum static friction force which represents the force needed to lift them out of it.

The researches of Vanossi[3] and Braun[9] on the FK models show that when strength K is small[3,10] and the system is in an underdamped state, the hysteresis of the system is obvious which is also convenient for the explanation of some problems in this article. In this paper, we focus on the effects of Gaussian colored noise in the underdamped[2,20] dynamics of a one-dimensional chain of interacting atoms sliding over a substrate potential. If not stated differently, the value $m = 1$, $K = 1$, and $\gamma = 0.7$ define our system units. $B_{\mathrm{f}} = (m\gamma)^{-1}$ represents the maximum asymptotic value of the chain mobility.[19,20]

3. Results and disussion

The length scale competition between the substrate and interatomic potentials controls the static and dynamic behavior of the system,[3,4,17] resulting in a rich complexity of spatially modulated structures for the chain particles. Following the previous studies in the FK models,[1–3] we have studied the incommensurate case ($b/a = 144/233$) and the commensurate

case ($b/a = 1$). For different values of the model parameters noise intensity D and the correlation time τ, we explore the behavior of the chain mobility as a function of variations of F. And the combined effects of noise intensity D and correlation time τ on the maximum static friction force F_s have also been investigated in detail.

3.1. Noise intensity effects

3.1.1. Incommensurate case ($b/a = 144/233$)

The behavior of the chain mobility B as a function of variations of the driving force F, for three different values of noise intensity D and fixed correlation times ($\tau = 1$, $\tau = 10$, and $\tau = 100$), is shown in Fig. 1, to investigate the effect of the noise intensity D. In this section, we consider the case of the incommensurate, and we choose $a = 1$, $b/a = 144/233$, $c = a/\beta = 144/89$, so that the system size is $L = 144$ and the chain is made up of $N = 233$ particles.[7,15]

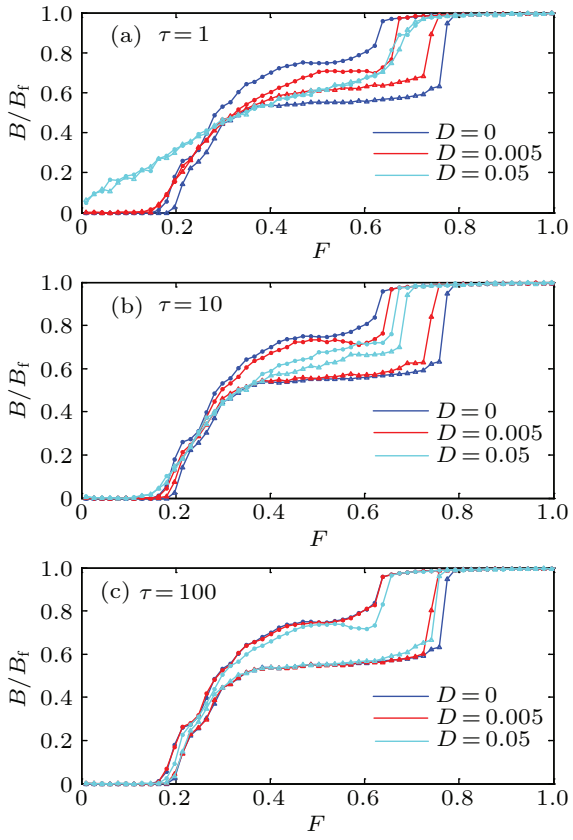


Fig. 1. Noise effects on static friction and hysteresis of the $B(F)$ characteristics for the incommensurate case when $D = 0, 0.005, 0.05$ for three cases: (a) $\tau = 1$, (b) $\tau = 10$, and (c) $\tau = 100$. Triangles and circles denote, respectively, the increasing and decreasing processes of F.

In Fig. 1(a), when noise intensity $D = 0$, a large hysteresis is clear. The larger value of noise intensity contributes to the disappearance of hysteretic and the decrease of the maximum static friction force F_s (when $D = 0$, $F_s \approx 0.18$; $D = 0.005$, $F_s \approx 0.15$; $D = 0.05$, $F_s < 0.017$), which indicates that the noise makes the atoms move along the chain much easier than themselves. Moreover, as the value of the F rises, the increase of D comes with a greater chain mobility B (when $F = 0.6$, $D = 0$, $B \approx 0.58$; $D = 0.005$, $B \approx 0.62$; $D = 0.05$, $B \approx 0.65$). Recent studies[19,20] of the one-dimensional FK models have demonstrated that noise excitation makes it easier for atoms to escape from the substrate potential. The results concluded from Fig. 1 also verify this view.

Figures 1(a) and 1(b) have a similar conclusion that is the hysteresis and maximum static friction F_s of the system decline as the noise intensity grows. The difference between Figs. 1(a) and 1(b) can be concluded that the increase of the correlation time τ renders a slower decline of the hysteresis and F_s. As shown in Fig. 1(c) ($\tau = 100$), the comparatively large value of the correlation time τ makes the hysteresis and F_s almost insusceptible to noise intensity. We can obtain from Fig. 1 that the greater the correlation time τ, the slower the decrease of the hysteresis and F_s. The result means that noise intensity has a positive effect on reducing hysteresis and F_s, whereas a change in correlation time will hinder this process.

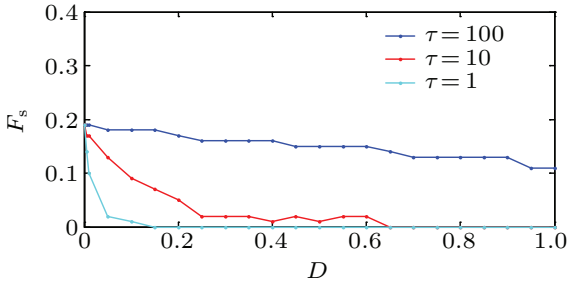


Fig. 2. Noise effects on maximum static friction force for the incommensurate case.

Figure 2 displays the detailed behavior of the maximum static friction force F_s with growing noise intensity D. The maximum static friction F_s drops as D increases. However, this trend varies depending on the correlation time. The variation is dramatic when $\tau = 1$ and invisible when $\tau = 10$. In particular, with appropriate parameters (when $D \approx 0.15$, $\tau = 1$), the system will give rise to super-lubricity. And the region, in which super-lubricity can happen, is marked in Fig. 3. However, there is no super-lubricity while the correlation time is too large ($\tau = 100$) which indicates that super-lubricity is possible for us if we choose appropriate noise parameters.

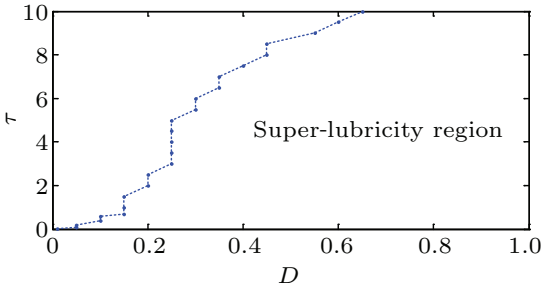


Fig. 3. Super-lubricity region for the incommensurate case.

Figures 1 and 2 show that for the incommensurate case, noise excitation makes it easier for atoms to escape from

the substrate potential and accelerate the motion of the system. With suitable noise intensity and correlation time, superlubricity happens. To verify the relevant conclusions in-depth, we have also carried out simulations for other irrational choices of the three characteristic lengths a, b, and c of the model.

3.1.2. Commensurate case ($b/a = 1$)

In this section, we shall focus on the hysteretic behavior of B as a function of F and the effect of noise intensity imposed on F_s for the case of a commensurate choice among the three model length scales already considered in a previous study.[19,20] Therefore, the numerical results refer to a substrate potential characterized by the parameters $a = 1$ and $c = a/\beta = 30/24$. The simulations are performed for a size $L = 140$ and a chain made up of $N = 140$ particles.[2,10]

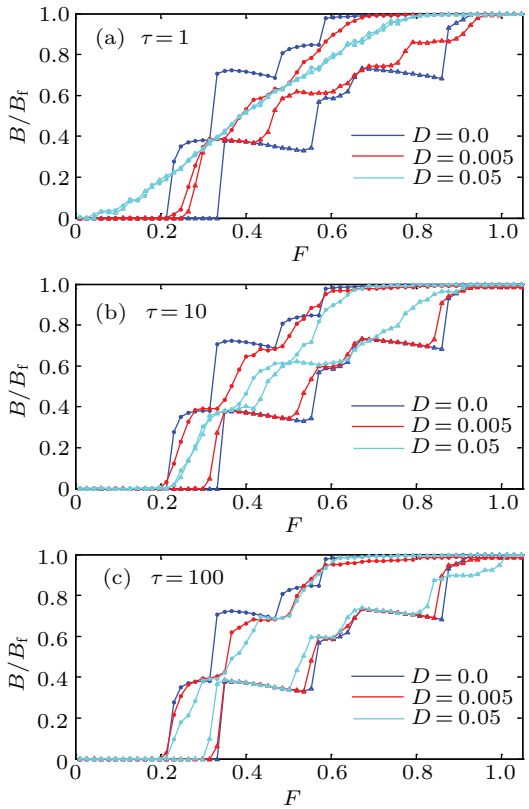


Fig. 4. Noise effects on static friction and hysteresis of the $B(F)$ characteristics for the commensurate case when $D = 0$, 0.005, 0.05 for three cases: $\tau = 1$, $\tau = 10$, and $\tau = 100$. Triangles and circles denote the increasing and decreasing process of F respectively.

Figure 4 shows the noise intensity D effects on the mobility-driving characteristics for a commensurate interface. In Fig. 4, when the correlation time is fixed, the width of the hysteretic region and the maximum static friction force F_s decrease to varying degrees due to the increase of D. This trend is less pronounced when the value of correlation time is large. Moreover, as shown in Fig. 4(a), the introduction of the noise accelerates the chain motion of the system as the force F rises (when $F = 0.6$, $D = 0$, $B \approx 0.6$; $D = 0.005$, $B \approx 0.63$; $D = 0.05$, $B \approx 0.8$), the greater the noise intensity, the greater the chain mobility. The relevant change diminishes with the increase of correlation time which can be observed from Figs. 4(b) and 4(c). As a result, the noise intensity tends to reduce the hysteretic region at finite correlation time, destroy the occurrence of parametric resonances inside the chain, and favor sliding with higher mobility values.

Conclude from Figs. 1(a) and 4(a): for a commensurate interface, the chain length is $L = 144$, and the number of atoms is $N = 233$, whilst an incommensurate case has the following $L = 140$ and $N = 140$. Albeit similar in chain length, despite having fewer atoms, when the commensurate interface has a noise intensity of $D = 0$, its hysteresis region and F_s are significantly larger in comparison. Figure 1(a) shows that the hysteresis and F_s vary by noise. The distinction between the two circumstances is that for the commensurate interface (Figs. 4 and 5), the atoms are more strongly coupled and entrapped by the substrate potential[5,10,19] so that the introduction of the noise make this coupling unstable and makes the atoms move along the chain much easier than before. Therefore, the influence is more vigorous for the commensurate case.

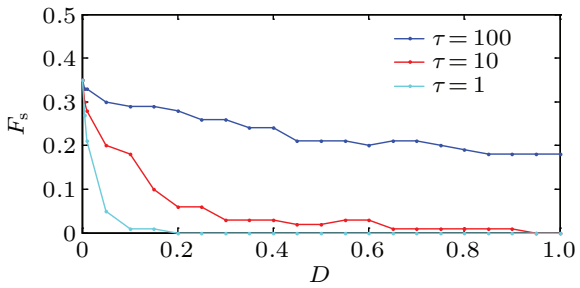


Fig. 5. Noise effects on maximum static friction force for the commensurate case.

The variation of the maximum static friction force F_s with respect to noise intensity D for the commensurate interface is plotted in Fig. 5. It is found that the increase of D contributes to the decrease of F_s. The shorter the correlation time τ, the more obviously F_s varies. Figure 6 depicts the region, in which the super-lubricity can appear. It is noteworthy that the system is much easier to give rise to super-lubricity for the incommensurate interface ($\tau \approx 0.01$, $D \approx 0.1$) than the commensurate interface ($\tau \approx 0.01$, $D \approx 0.1$).

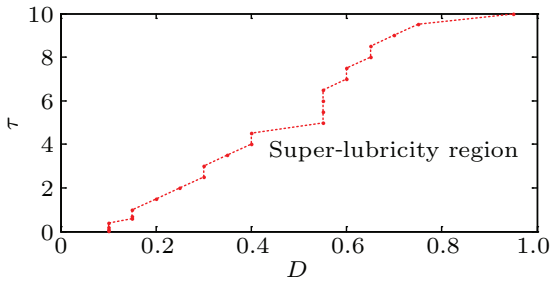


Fig. 6. Super-lubricity region for the commensurate case.

3.2. Correlation time effects

The above simulation results indicate that the hysteretic and maximum static friction force F_s depends notably on the correlation time τ. In order to study the effect of the correlation time on the nano-friction phenomena in more detail, we plot the variation of the $B(F)$ for different values of correlation time τ with different noise intensities D. Meanwhile, the maximum static friction force F_s with respect to correlation time τ is given. This section is divided into the incommensurate case and the commensurate case.

3.2.1. Incommensurate case ($b/a = 144/233$)

In this section, we have considered the case of the incommensurate, so we choose $a = 1$, $b/a = 144/233$, $c = a/\beta = 144/89$, so that the system size is $L = 144$ and the chain is made up of $N = 233$ particles.[2,7]

As depicted in Fig. 7, for the incommensurate case, the correlation time has a clear effect on the hysteresis and maximum static friction force F_s. And the hysteretic region tends to increase with increasing values of correlation time τ, and the correlation time also affects the maximum static friction force F_s (in Fig. 7(a), $\tau = 0.1$, $F_s \approx 0.11$; $\tau = 1$, $F_s \approx 0.15$; $\tau = 10$, $F \approx 0.17$). Figures 7(a) and 7(b) demonstrate similar conclusion, however, under the fixed noise intensity D, the trend of increasing the hysteretic region and F_s are different due to different correlation time.

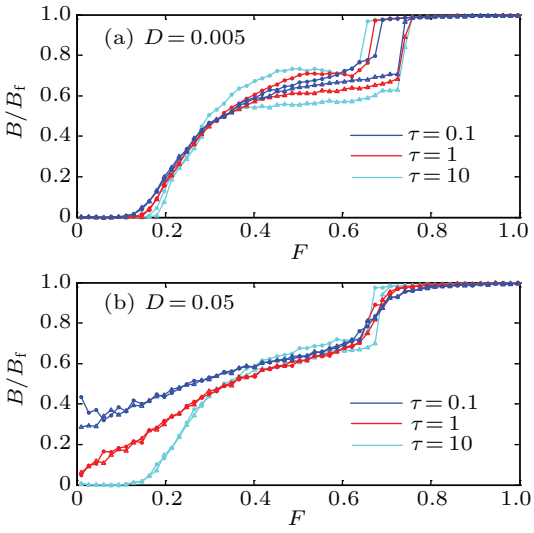


Fig. 7. Correlation time on static friction forces as well as the hysteresis for the incommensurate case, in which triangle and circle denote the processes of increasing and decreasing external forces depicting the hysteresis behavior for two cases: (a) $D = 0.005$, (b) $D = 0.05$.

Figure 8 displays the detailed behavior of the maximum static friction force F_s with the change of correlation time τ at different noise intensity D. F_s is increased as τ grows, and eventually reaches a relatively stable value ($D = 0.005$, $F_s \approx 0.18$; $D = 0.05$, $F_s \approx 0.17$). The difference between the two situations ($D = 0.005$, $D = 0.05$) is that the greater the noise intensity, the more sharply the increase. The results mean that the correlation time encourages the increase of the hysteresis and the maximum static friction force F_s, however, the noise intensity plays the opposite role. The findings summarized in Figs. 7 and 8 verify some of the conclusions in Subsection 3.1.

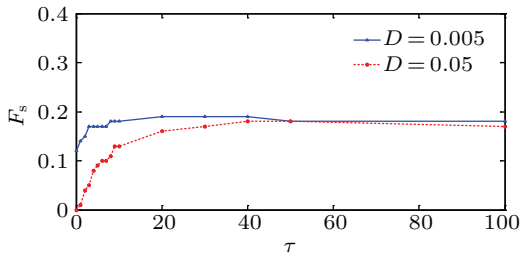


Fig. 8. Correlation time on maximum static friction force for the incommensurate case.

3.2.2. Commensurate case ($b/a = 1$)

In order to further study the effect of the correlation time on the nano-friction phenomena, this section investigates the commensurate case. Therefore, the numerical results refer to the substrate potential characterized by the parameters $a = 1$ and $c = a/\beta = 30/24$. In this case, the chain length $L = 140$ and the number of atoms $N = 140$.

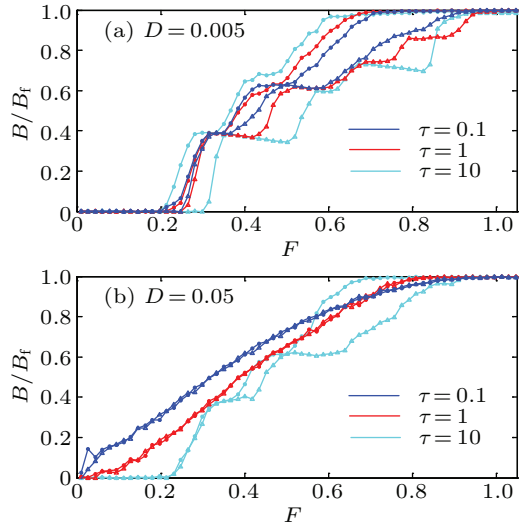


Fig. 9. Correlation time effects on static friction and hysteresis of the $B(F)$ characteristics for the incommensurate case, when $\tau = 0.1$, 1, 10 for two cases: (a) $D = 0.005$, (b) $D = 0.05$.

Figure 9 gives the process of the hysteretic behavior in the characteristics B *versus* F for the commensurate interface. It is shown that for given values of noise intensity D (where $D = 0.005$, 0.05 respectively), with the increase of the correlation time τ, the region of the hysteretic is increased. Meanwhile, the maximum static friction force F_s goes up with increasing the correlation times (in Fig. 9(a), $\tau = 0.1$, $F_s \approx 0.25$; $\tau = 10$, $F_s \approx 0.3$). To sum up, the difference between the Figs. 9(a) and 9(b) is the increased tendencies of the hysteresis region which is related to noise intensity D.

For the commensurate case, the variation of the maximum static friction force F_s with respect to correlation time τ for

different noise intensities D is plotted in Fig. 10. The maximum static friction force F_s increases to a relatively stable value ($D = 0.005$, $\tau \approx 0.33$; $D = 0.05$, $\tau \approx 0.31$) while τ increases. The greater the noise intensity, the more evident the increase.

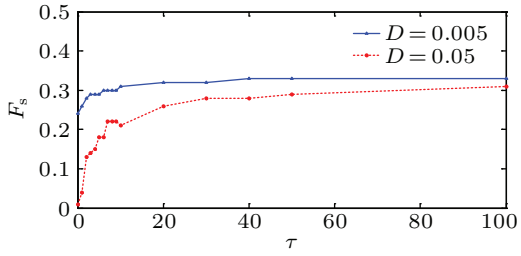


Fig. 10. Correlation time on maximum static friction force for the commensurate case.

It is summarized from Figs. 7–10 that for commensurate interface, the influence of colored noise on hysteresis and F_s is more evident. From what we have mentioned above, noise intensity $D = 0.05$, correlation time rises from $\tau = 0$ to $\tau = 10$, hystersis region (Figs. 7(b) and 9(b)) and the maximum friction (Figs. 6 and 8) both experienced the processes from appearing to growing. However, difference also exists. Given the larger increase of F_s from 0 to 0.31 for commensurate interface (Fig. 7(b), $\tau = 10$) and from 0 to 0.17 for incommensurate case (Fig. 5(b), $\tau = 10$) and wider hysteresis area for the former interface, it is easy to conclude that noise poses a more significant effect on hysteresis and F_s for commensurate case.

4. Conclusions

In this paper, we have investigated the effects of Gaussian colored noise on a one-dimensional chain of interacting atoms driven by an external force. Starting from the two geometrically opposite ideal cases of commensurate and incommensurate interface. In particular, we have focused our study on the variation regularity of the hysteretic behavior and the maximum static friction force which are affected by the Gaussian colored noise.

The results indicate that the noise intensity has a positive effect on reducing hysteresis and F_s, whereas the change in correlation time hinders this process. In particular, suitable correlation time and noise intensity give rise to super-lubricity. The difference between the two circumstances is that for the commensurate mating contacts, the influence of the noise is much stronger in terms of triggering the motion of the FK model than for the incommensurate interface since the atoms in the former case are coupled and entrapped more strongly by the substrate potential. We hope that the results presented in this work may be relevant to future theoretical and experimental studies concerning microscopic tribology of the real physical systems, where the geometrical features of the interfaces in relative motion could play a major role.

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