Hysteretic behaviour in driven Frenkel–Kontorova chains on irregular substrates

2004 J. Phys.: Condens. Matter 16 S2895

(http://iopscience.iop.org/0953-8984/16/29/004)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **16** (2004) S2895–S2903 PII: S0953-8984(04)80329-1

Hysteretic behaviour in driven Frenkel–Kontorova chains on irregular substrates

A Vanossi, G Santoro and V Bortolani

INFM-S3 e Dipartimento di Fisica, Università di Modena e Reggio Emilia, Via Campi 213/A, 41100 Modena, Italy

Received 4 May 2004
Published 9 July 2004
Online at stacks.iop.org/JPhysCM/16/S2895
doi:10.1088/0953-8984/16/29/004

Abstract

The hysteretic dynamics of a Frenkel–Kontorova chain subject to irregular substrate potentials and driven by an external dc force is studied both in the underdamped and in the overdamped regime at zero temperature. The choice of a rigid external potential defined by the sum of two sinusoidal functions with different periodicity allows us to simulate microscopic sliding over quasiperiodic and multiple-well periodic substrates. We analyse, for different parameter values of the model, the behaviour of the centre of mass average velocity of the chain as a function of an adiabatic increase and decrease of the applied driving. For small damping coefficients (negligible dissipative forces), at a fixed value of the substrate potential amplitude, the width of the hysteresis region is markedly influenced by the chain stiffness. As expected, in the overdamped dynamical regime no hysteresis is observed. We comment on the nature of the dynamical states displayed during the chain motion at different strengths of the dc driving.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Nonlinear systems driven far from equilibrium exhibit a variety of complex spatial and temporal behaviours. In particular, in the emerging field of nanoscale sciences and technologies [1], understanding the nonequilibrium dynamics of simple nonlinear particle arrays and clusters subjected to a substrate potential, viscous damping and driven by an external force, is becoming more and more often a central issue.

It has recently been shown [2] that simple phenomenological models of friction, which are typically low dimensional compared to the large number of degrees of freedom available in the array, give reasonable agreement with experimental results on nanoscale tribology, being able to capture the main features of the complicate dynamics involved. In particular, there has been a growing interest in *driven* Frenkel–Kontorova (FK) models [3], in which a certain

density of interacting particles is made to slide, by the application of an external driving force and in the presence of dissipation, over a rigid substrate.

The shape of the substrate potential, assumed purely sinusoidal in the *standard* FK chain [4], is a factor of significant importance when modelling physical systems. The deviation from the periodic sinusoidal shape modifies the parameters of both linear and nonlinear interactions, leading to qualitatively different features such as the appearance of different types of kinks, phonon branches, changes in kink–antikink collisions, and modification of breather (kink–antikink bound state) solutions. All of these characteristics may lead to a consequent drastic change in the friction dynamics between the two solid interfaces in relative motion.

In this paper, we consider the dynamics of a driven FK chain subject to an on-site potential defined by the sum of two sinusoidal functions with different periodicity [5, 6]. The incommensurate or commensurate choice among the system length-scales allows us to simulate the motion of the system over quasiperiodic or multiple-well periodic substrates, respectively. In particular, we focus on the hysteretic behaviour [7] of the chain average velocity as a function of the adiabatically applied driving force at zero temperature. As long as the thermal energy is much smaller than the amplitude of the external potential the qualitative dynamical behaviour does not change much and an analysis in the absence of a an external noise, such as thermal fluctuations (via a Langevin equation approach), is reasonable, as shown through numerical simulations of similar models [8]. Regarding this point, it seems often relevant that the system has many degrees of freedom. In the case for example of just one (Brownian) particle [9] the hysteresis phenomenon disappears even for an infinitesimally small noise amplitude, because the fluctuations can kick the particle out of a locked state.

In the velocity–driving characteristics, the kinds of transitions between pinned, intermediate and sliding states, for adiabatically increasing and decreasing force, do not have to occur at the same value of the applied driving. The behaviour depends strongly on whether the system degrees of freedom have inertia or if the inertia is negligible compared to dissipative forces [10]. In the presence of strong dissipation, when the viscous friction coefficient γ is much larger than the characteristic vibrational frequency at the bottom of the substrate potential, the motion is *overdamped*; the pinning–depinning transition is in most cases expected to be of second order, and indistinguishable from the reverse one. Interesting results were obtained by reducing the time-independent Smoluchowski equation for a steady state of the driven system to a one-particle equation with an effective on-site potential, which then was solved numerically by a transfer operator technique [11]. The results show the existence of a nonlinear mobility region, but without any bistability phenomenon. If, on the other hand, the motion is *underdamped*, we expect that hysteresis is possible because the inertia can overcome a pinning centre.

The paper is organized as follows. In section 2 we briefly describe the main features of the damped, driven FK model subject to the on-site potential defined by the sum of two sinusoidal functions with different periodicity. We summarize the numerical technique implemented to solve the nonlinear equations of motion and to study the hysteresis cycle. Sections 3 and 4 are devoted to the presentation of the simulation results for quasiperiodic and multiple-well periodic substrate potentials, respectively, both in the underdamped and overdamped dynamical regimes. Conclusions are given in the last section.

2. The model

We investigate the dynamics of a driven FK model whose N particle positions $\{x_i\}$ satisfy the following equations of motion:

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

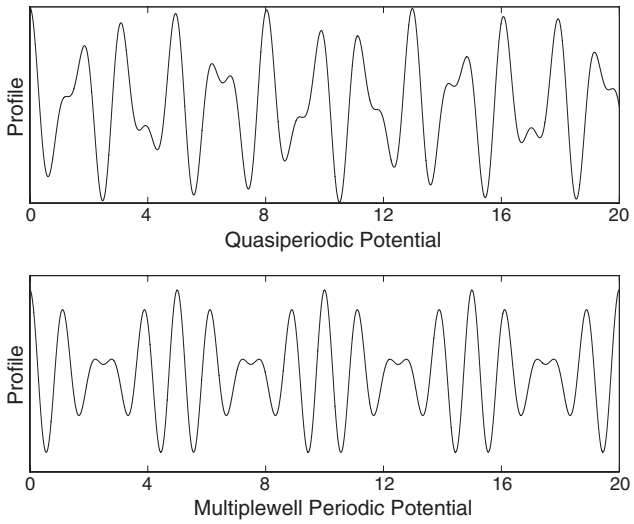

Figure 1. Profiles of the substrate potential for the *golden-mean* quasiperiodic case (upper panel) and the $\beta = 24/30$ multiple-well periodic case (lower panel). Only a limited portion of the system length is displayed for clarity.

where γ is a phenomenological viscous damping. This coefficient can be thought of as representing degrees of freedom inherent in real, physical systems which are not explicitly included in our model (e.g., vibrational or electronic excitations in the substrate). In a 2D isotropic elastic model with no extrinsic damping terms, it has been recently shown [12] that, at least qualitatively, the dynamical behaviour observed is similar to that seen in simple 1D friction models including ad hoc viscous damping [13]. In equation (1) the dots denote time derivatives and F represents the external driving force applied to all atoms of the chain. The numerical simulations are carried out choosing for the interatomic interaction a Morse-type potential

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

with strength K and natural equilibrium spacing $b = L/N$, where L is the chain length. The geometry of the substrate potential is defined via the values of the two spatial periodicities a and $c = a/\beta$. In order to avoid effects due to the boundary layers, the periodic boundary conditions

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

are imposed on the system.

The length scale competition between the substrate and the interatomic potentials controls the static and dynamic behaviour of the system, resulting in a rich complexity of spatially modulated structures for the chain particles. In this paper, we focus on the hysteretic response of the FK chain to the imposed external driving both for *mutually incommensurate* (quasiperiodic substrates) and *mutually commensurate* (multiple-well periodic substrates) choices of the three characteristic lengths a, b and c of the system. The two panels of figure 1 show a portion of the substrate potential profiles considered for simulations.

A fourth-order Runge–Kutta algorithm is implemented to solve numerically the equations of motion (1). The system is initialized with the particles placed at rest at uniform separation b. The dc-force, F, is then increased adiabatically. For every value of F, equation (1) is integrated

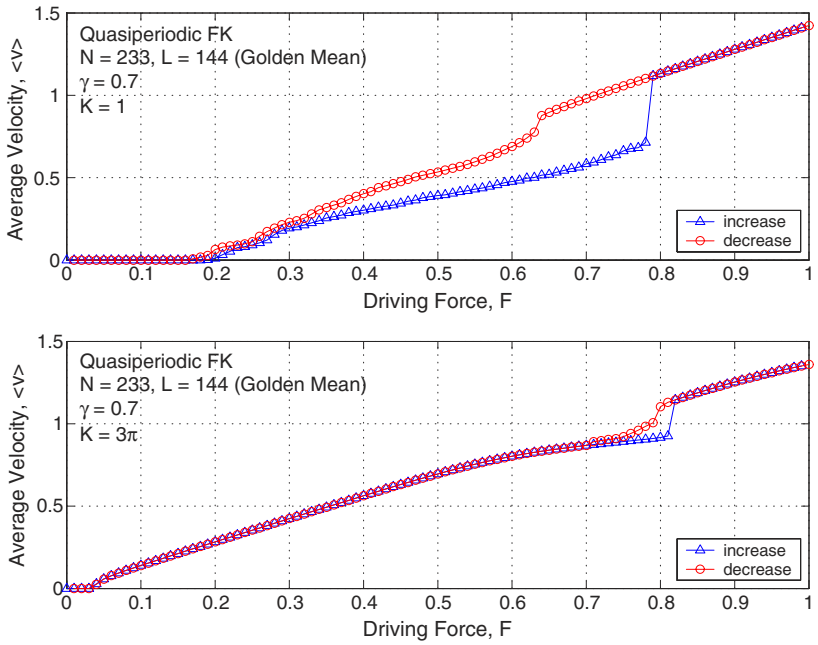

Figure 2. $\langle v\rangle$–F characteristics for two different values of the interparticle interaction strength K (chain stiffness). The two distinct symbols, corresponding to an adiabatic increase (triangle) and decrease (circle) of the applied driving, show the occurrence of the hysteretic behaviour. The simulations refer to the *underdamped* case of a *quasiperiodic* FK chain with inherent lengths related by the golden mean winding number.

over a time period $[0, T]$ long enough to eliminate transient behaviour and reach a steady state for which the centre of mass average velocity of the chain $\langle v\rangle$ is then calculated. The final chain configuration (positions and velocities) obtained at one value of F is used as the initial condition for the integration of the dynamics for the next value of the driving. In order to analyse the backward transitions from running to locked states and the hysteresis cycle, we adopt the same numerical procedure by decreasing adiabatically down to zero the applied force F.

3. Quasiperiodic substrates

In figure 2 we show the centre of mass average velocity of the chain as a function of the imposed driving for an *underdamped* dynamical regime ($\gamma = 0.7$). Here, we have considered the case of the familiar *golden mean* winding number. We recall [5] that the presence of periodic boundary conditions forces us to approximate the desired incommensurate numbers by ratios of integers. For our choice, the system lengths a, b and c turn out to be related by ratios of Fibonacci numbers. In particular, we have chosen $a = 1$, $b = 144/233$ and $c = a/\beta = 144/89$, so that the system size is $L = 144$ and the chain is made up of $N = 233$ particles. In the panels of figure 2, corresponding to two distinct values of the interatomic interaction strength K, the existence of the hysteretic behaviour in the $\langle v\rangle$ versus F curves is highlighted by the two different symbols used for the adiabatic increase (triangles) and decrease (circles) of the force. In the *upper* panel, when the external driving is increased, it is possible to distinguish roughly three different regions. Below a critical value $F_s \approx 0.2$ (*static friction*),

the applied force is too low and the atoms, trapped in the external quasiperiodic potential wells, do not move. The system is in the *locked* (or *pinned*) *state* with a zero mobility. Above F_s, the motion starts via the formation of a small number of isolated, narrow defects (*kinks*) along the chain. These states correspond to an *intermediate-sliding* regime, where a detailed study of the particle trajectories indicates clearly that the local compression zones are moving but not the individual atoms, except when a kink passes through their site. Physically this phenomenon signifies that it is easier to move a dislocation coherently along the chain than to move all the atoms simultaneously. The number of these kinks increases as one raises the driving force, until they begin to overlap. At a second thresholds force ($F_r \approx 0.79$), the chain dynamics changes to the high driving running regime. In this case, all the particles slide, almost uniformly, over the quasiperiodic substrate. These states, also called *solid-sliding* states, are characterized by the largest average sliding velocities $\gamma\langle v\rangle = F$.

When the external field is adiabatically reduced, the system leaves the last solid-sliding state, reaching the intermediate regime of motion, at a force F ($\approx$0.63) lower than F_r. As the chain is either in an intermediate-sliding state or in a solid-sliding state, depending on its initial velocity condition, the system exhibits bistability and the transition between these two regimes shows hysteresis. The kinetic energy being much larger than the thermal energy, the introduction of a finite (not to high) temperature should not modify this scenario seriously. One may expect that the transition between the high running state and the intermediate sliding regime will be simply smeared out. Then for forces $F < 0.16$ ($<F_s$) the chain drops back to the pinned state. In the *lower* panel of figure 2, the same characteristic curves of $\langle v\rangle$ as a function of F are displayed for a much stiffer chain, that is, for a larger value of the interatomic interaction strength K. In this situation, even just above F_s, there is an appreciable background drift velocity on the top of which the inhomogeneities occur and we observe, from the very beginning, a relatively large chain velocity (i.e. $\langle v\rangle \sim F/\gamma$). For these values of the model parameters, the width of the hysteretic region decreases considerably and manifests itself just in the neighbourhood of the parametric resonances [14].

Figure 3 shows the $\langle v\rangle$ versus F characteristics for the *overdamped* dynamics ($\gamma = 3$) of the quasiperiodic FK chain. As already mentioned, the transition from the locked to the running state is expected to be of second order, and indistinguishable from the backward process. In this case, both for the soft ($K = 1$, upper panel) and the stiff ($K = 3\pi$, lower panel) chain, the particle inertia is negligible compared to dissipative forces. The system does not show evidence of any bistability phenomenon and, consequently, the hysteresis region is missing. As in the previous underdamped regime and in accordance with the theoretical consideration based on the *standard* FK model, we observe that, for the same substrate potential amplitude, the static friction value drops as the chain stiffness (i.e. K) increases. Obviously, the value of the viscous damping coefficient γ does not affect F_s.

We have also carried out simulations for other irrational choices of the characteristic lengths a, b and c of the model. For all these simulations, we have recovered an hysteretic dynamical behaviour consistent with the already mentioned observations.

4. Multiple-well periodic substrates

In this section, we shall focus on the hysteretic behaviour of $\langle v\rangle$ as a function of F for the case of a commensurate choice among the three model length scales already considered in a previous study [6]. Therefore, the numerical results refer to a substrate potential characterized by the parameters $a = 1$ and $c = a/\beta = 30/24$. This potential has a periodicity $T = 5$ and we count five wells, with different amplitudes, in each substrate unit cell. The simulations are performed for a system size $L = 30$ and a chain made up of $N = 30$ particles. The effect of the external driving is to tilt the potential, producing a corrugated surface whose average slope

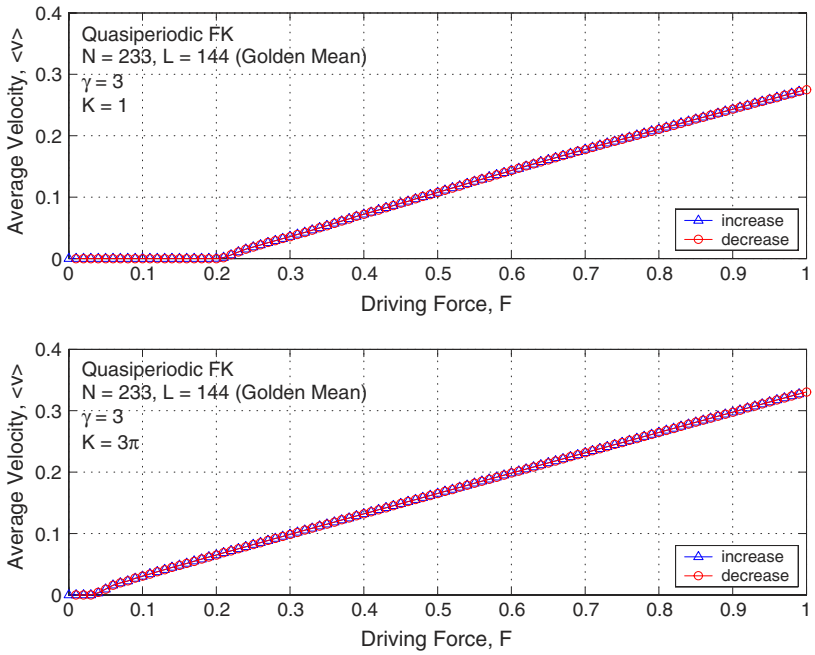

Figure 3. $\langle v\rangle$–F characteristics for the same *quasiperiodic* FK model of figure 1, but in the *overdamped* regime. Adiabatic increase and decrease of the force are denoted by triangles and circles, respectively. In this case, independently of K, no hysteresis is observed.

is determined by F. Increasing the driving leads, in the presence of an *irregular* substrate, to a *sequential* disappearance of the potential minima. Thus, as already pointed out [6], one should distinguish in this case between a *static* ($F = 0$) and a *dynamic* ($F \neq 0$) commensurability of the coverage variable (defined as the ratio of the number N of atoms to the number of minima in the substrate potential).

Figure 4 represents the centre of mass average velocity as a function of the driving in the *underdamped* dynamical regime. The upper ($K = 1$) and lower ($K = 3\pi$) panels clearly show an hysteretic behaviour in the characteristics $\langle v\rangle$ versus F. Because of the complex nature of the substrate potential, as compared for example to the simple sinusoidal one of the standard driven FK model, it is not easy to trace a precise relation between the multiple steps displayed in these curves, above the depinning threshold F_s, and the various dynamical behaviours observed during the chain motion. These regimes correspond to rearrangements of particle configurations (spatial inhomogeneities) with distinct periodicities and amplitudes. When these commensurate moving structures are extended enough with respect to the substrate period, their topological shape turns out to be decorated by superimposed smaller deformable particle configurations with the same periodicity T. Their geometries and amplitudes are, clearly, dependent also on the stiffness (i.e. the interatomic strength K) and length (i.e. the particle number N) of the chain. Comparing the lower panel of figure 4 to the upper one, it can be noted that the spatially inhomogeneous intermediate states, between the locked configuration and the solid-sliding one, tend to decrease in number since the relative separations among particles are more constrained by the higher chain stiffness.

As before, in this underdamped regime the dissipative forces are negligible compared to the particle inertia and the system, depending on its initial velocity, exhibits bistability with a hysteresis region whose width decreases for increasing values of K. In our simulations,

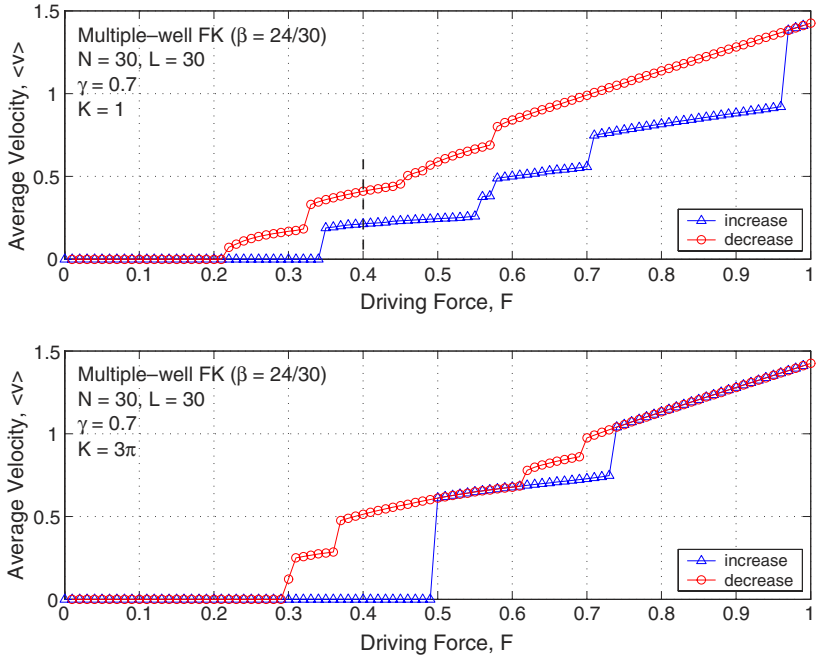

Figure 4. $\langle v \rangle$–F characteristics for the *underdamped multiple-well periodic* FK chain. Other model parameters are as shown. The black dashed vertical line at $F = 0.4$, in the upper panel, marks the two dynamical states of the chain displayed in figure 4.

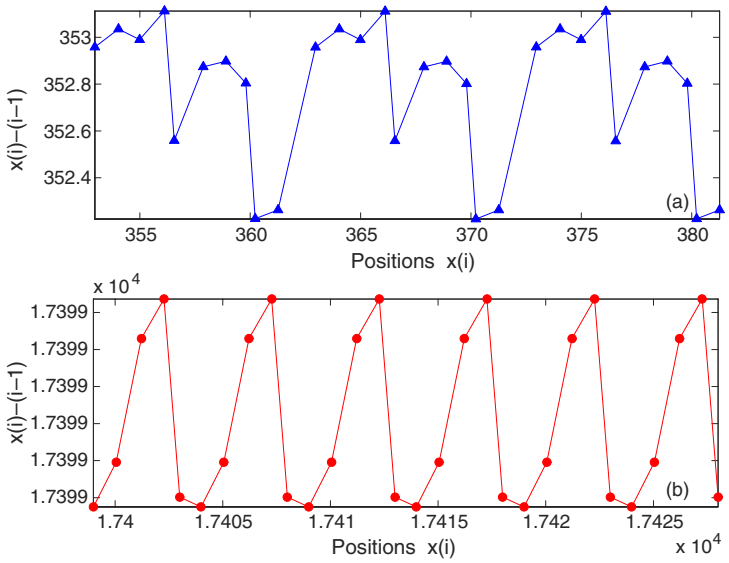

Figure 5. *Commensurate dynamical structures* of different periodicity and amplitude, corresponding to the two states at $F = 0.4$ indicated by the vertical dashed line in the upper panel of figure 3.

we have analysed some of the two dynamical states of the chain associated with the same value of the applied driving. In figure 5, we show the snapshots of the commensurate moving

structures occurring at a force $F = 0.4$. (The two states considered are those marked by the vertical dashed line in the upper panel of figure 4.) In plot (a) (adiabatic increasing process) we observe the dynamics of a ten-period structure with a calculated average amplitude around 0.91; plot (b) (adiabatic decreasing process) is instead characterized by a five-period structure with average amplitude equal 0.54. The values of these amplitudes can be an indirect measure of the degree of internal vibrational motion among particles. The solid-sliding regime, for example, is characterized by the dynamics of structures with approximately vanishing amplitudes, so that the motion is almost uniform.

We have also verified that very similar results are obtained considering the hysteresis of a bigger system ($L = 140$, $N = 140$), but with an identical substrate spatial geometry ($a = 1$, $c = a/\beta = 30/24$). In this case, therefore, a size-dependent effect seems to be excluded.

As in the previous section, we have checked that, also for the multiple-well periodic potential, the *overdamped* dynamics does not reveal any bistability phenomenon.

5. Conclusions

In this paper, we have investigated the *sliding dynamics* of an interacting chain of atoms subject to a dissipative viscous damping and driven by an external dc force over irregular substrate potentials. The choice of an on-site potential defined by the sum of two sinusoidal functions with different periodicity allows us to simulate the microscopic friction dynamics over quasiperiodic and multiple-well periodic substrates. In particular, we have focused our study on the hysteretic behaviour of the centre of mass average velocity of the chain as a function of the adiabatically increasing and decreasing driving, at zero temperature. This investigation has been carried out for different values of the model parameters. In the underdamped regime, we have observed a critical dependence of the width of the hysteretic region on the chain stiffness. At larger values of the interparticle interaction strength K, for example, hysteresis manifests itself just in the neighbourhood of the parametric resonances. On the other hand, for a large viscous damping coefficient (overdamped regime), the dissipative forces become predominant with respect to the inertia of the particles. The system no longer exhibits bistability, and the transitions between the different sliding states occur at the same value of the applied force. We have also commented on the nature of the distinct dynamical states giving rise to the multiple-steps feature in the $\langle v \rangle$ versus F curves.

The interesting temperature effects on the hysteresis behaviour of the model could be certainly evaluated in the framework of a Langevin-type dynamics. However, we expect that, as long as the thermal fluctuations are much smaller than the amplitude of the external potential, the qualitative dynamical response does not change significantly (simply smoothing the sharpness of the transitions) and an analysis in the absence of a an external noise is reasonable.

We hope that the results presented in this work may be relevant to future theoretical and experimental studies concerning microscopic tribology of real physical systems, where the geometrical features of the interfaces in relative motion (e.g., quasicrystal surfaces or lattices with a complex unit cell) could play a major role.

Acknowledgments

We are grateful to A R Bishop for valuable discussions. This work has been partially supported by INFM project PRA ‘Nanorub’.

References

[1] Persson B N J 2000 *Sliding Friction: Physical Principles and Applications* (Berlin: Springer)
Brushan B 2002 *Introduction to Tribology* (New York: Wiley)

[2] Rozman M G, Urbakh M and Klafter J 1996 *Phys. Rev. Lett.* **77** 683
Zaloj V, Urbakh M and Klafter J 1998 *Phys. Rev. Lett.* **81** 1227
Persson B N J 1997 *Phys. Rev.* B **55** 8004

[3] Braun O M and Kivshar Y S 1998 *Phys. Rep.* **306** 1
Braun O M and Kivshar Y S 2004 *The Frenkel–Kontorova Model: Concepts, Methods, and Applications* (Berlin: Springer)

[4] Aubry S 1983 *Physica* D **7** 240
Peyrard M and Aubry S 1983 *J. Phys. C: Solid State Phys.* C **16** 1593
Aubry S and Le Daeron P Y 1983 *Physica* D **8** 381

[5] Vanossi A, Röder J, Bishop A R and Bortolani V 2001 *Phys. Rev.* E **63** 017203

[6] Vanossi A, Röder J, Bishop A R and Bortolani V 2003 *Phys. Rev.* E **67** 016605

[7] Braun O M, Dauxois T, Paliy M V and Peyrard M 1997 *Phys. Rev. Lett.* **78** 1295
Braun O M, Bishop A R and Röder J 1997 *Phys. Rev. Lett.* **79** 3692

[8] Braun O M, Dauxois T, Paliy M V and Peyrard M 1997 *Phys. Rev.* E **55** 3598
Persson B N J 1993 *Phys. Rev.* B **48** 18140

[9] Risken H 1984 *The Fokker–Planck Equation* (Berlin: Springer)

[10] Strunz T and Elmer F-J 1998 *Phys. Rev.* E **58** 1612

[11] Trullinger S E, Miller M D, Guyer R A, Bishop A R, Palmer F and Krumhansl J A 1978 *Phys. Rev. Lett.* **40** 206
Trullinger S E, Miller M D, Guyer R A, Bishop A R, Palmer F and Krumhansl J A 1978 *Phys. Rev. Lett.* **40** 1603

[12] Röder J, Bishop A R, Holian B L, Hammerberg J E and Mikulla R P 2000 *Physica* D **142** 306

[13] Röder J, Hammerberg J E, Holian B L and Bishop A R 1998 *Phys. Rev.* B **57** 2759

[14] Strunz T and Elmer F-J 1998 *Phys. Rev.* E **58** 1601