Applications of Molecular Dynamics Simulations in two Dimensional Frenkel-Kontorova Model

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Abstract—Based on the molecular dynamics simulation, this manuscript is dedicated to the studies of dynamical behavior in the two dimensional Frenkel-Kontorova model with triangular symmetric periodic substrate when a dc drive and a circular ac driven force are applied. The numerical results show that the velocity of system increases in quantized steps with step weights of <V>=n (0,1,2,3…). This ensures the reliability and accuracy of the scheme of our molecular dynamics code. As an important application, it is also obtained from our numerical results that the critical depinning force (known as the static frictional force in the tribology) can be strongly affected by the direction of the dc force. The obtained results show that the static frictional force is minimum value for α=0^0 and 60^0. It are also noted that the curves are symmetric about α=30^0.

Keywords-component; molecular dynamics; Frenkel-Kontorova model; dc force; Runge-Kutta algorithm; superconducting devise

I. INTRODUCTION

Computational simulation and modeling of complex many-body system is a very advanced field, the importance of which increases strongly. This great filed is attributed to the enormous progress in computer technology as well as in the progress of theoretical concepts and models. In some cases, the accuracy and reliability are good agreement with experiment. The computer becomes the virtual laboratory in which a system is studied- a numerical experiment. One of the advantages of computational simulations is that all the parameters are well defined and their influences on the results can be analyzed. By that, computational-theoretical modeling and algorithm becomes a powerful tool for predicting yet unknown properties, and suggesting experiments.

Molecular dynamics (MD) simulation provides the methodology for detailed microscopic modeling on the molecular scale[1,2]. In the classical N-body problem, there lacks a general analytical solution, the only path open is the numerical one. The continually increasing power of computers makes it possible to pose questions of greater complexity, with a realistic expectation of obtaining meaningful answers. Computer programs are an important part of any MD project and feature prominently among the recipes. By the way, a computer program is merely the statement of an algorithm, which is a mathematical procedure. As the important applications, MD numerical simulations are to be found in physics, chemistry, biochemistry, materials science, and in branches of engineering[3,4].

Given the near ubiquity of MD, in order to gain an insight into the complex macroscopic many-body systems with competing interactions, attention has been always focused on simple many-body models. Among these models, the Frenkel-Kontorova (FK) model is one of the simplest but still complexly enough to capture the essence of many physical and biological phenomena[5,6]. The standard FK model represents a chain of harmonically interacting particles subjected to a sinusoid substrate potential. In order to

explain some complex macroscopic phenomena, such as charge density or spin density wave conductors[7,8], vortex lattices[9], Josephson-junction arrays[10], and superconducting nanowires[11], a large number of works have been studied by computer simulations of MD[12-16]. For example, Using molecular dynamics simulation, Flor á et al. have studied in detail the overdamped dynamics of the 1D FK model submitted to the ac and dc drives the staircase macroscopic response in the curve of average velocity as a function of the average external driving force has been obtained in the references[17-19]. The dynamical hull function that describes the driven structure becomes non-analytical above the transition point, and the result of this is the dynamical locking at certain resonant values. The dynamical mode locking and the dynamical Aubry transition for the commensurate and IC structure, respectively, appear to be one of the universal feature of the systems with the competition of time scales in the ac-driven dynamics. Recently, the influence of the amplitude and frequency of the external ac force on the interference phenomena of the FK model has been studied in the works of Hu et al.

The simple 1D FK model, being very useful in understanding the above-mentioned phenomena, has been qualitatively explained. However, in practice, in order to reproduce the feature more adequately and to include subtler details which can be realized in experiments, it is necessary to generalize this mode to the two dimensional (2D) case, where it would be possible for the sliding particle to avoid passing over a highest barrier in the substrate potential, which they has to overcome in the 1D case. In the application of rachet and interference phenomena, the effect on the dynamics of the many-body system, especially on the transport properties of the 2D driven FK model, has not been investigated any further even if it is of great importance.

Based on MD numerical simulation, the aim of this manuscript is dedicated to the studies of dynamical behavior in the two dimensional Frenkel-Kontorova model with triangular symmetric periodic substrate when a dc drive and a circular ac driven force are applied. The numerical results could provide theoretical guidance for future experiment and application of lattice dynamics.

II. NUMERICAL CALCULATION METHOD

We study the dynamical behavior for a 2D lattice of particles with interaction coupled to a periodic substrate potential with the triangular symmetry. For simplicity, in the FK model, the substrate potential is taken as a sinusoidal function (shown in Fig.1),

$$V_{sub} = -f(\cos\frac{2\pi y}{a_y} + \cos\frac{2\pi(\sqrt{3}x - y)}{\sqrt{3}a_x} + \cos\frac{2\pi(\sqrt{3}x + y)}{\sqrt{3}a_x} \quad (1)$$

where $a_x = a$ and $a_y = \frac{\sqrt{3}a}{2}$ are the lattice constants, f is the magnitude of the adhesive force between the two layers.

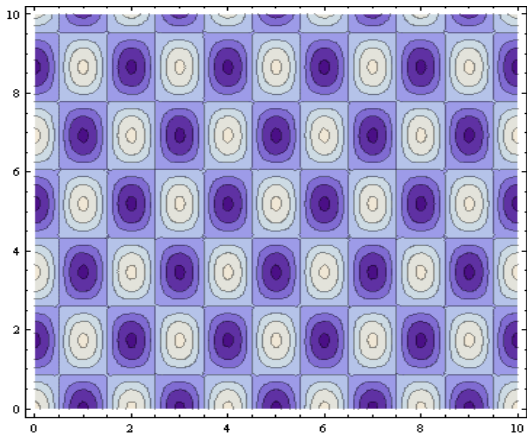

Figure 1. Schematic view of the substrate potential.

We consider an arbitrary particle of (i,j) in the upper layer which interacts with the six nearest neighbors. We also consider the case of the simplest harmonic interaction between the particles in the upper layer

$$V_{\text{int}} = \sum_{i,y} \frac{K}{2}(r_{i,j} - l_0)^2 \quad (2)$$

with a stiffness strength K. The lattice constants of the upper layer is $l_0 = a$.

We consider the dynamics of an arbitrary particle with positive vector $r_{i,j} = (x_{i,j}, y_{i,j})$. The equation of motion of an arbitrary is given as follows:

$$\dot{r_{i,j}} = -\frac{\partial(V_{sub} + V_{\text{int}})}{\partial r_{i,j}} + F(t) \quad (3)$$

In the 2D FK model, the system is driven by dc and ac force, i.e., $F(t) = F_{dc} + F_{ac}$. The dc driven force $F_{dc} = (F_{ext}\cos\alpha, F_{ext}\sin\alpha)$ is applied for each particle with α being the angle between Fext and the unit vector of x axis. Meanwhile, the ac driven force is $F_{ac} = F_{ac}\sin(2\pi\mu)x + F_{ac}\cos(2\pi\mu)y$, where F_{ac} is the magnitude of the ac drive and μ is the frequency of the ac drive.

The following scheme is implemented in the fourth-order Runge-Kutta algorithm to numerically solve Eq.(3) with the periodic boundary conditions. The dc force F_{dc} is varied with the step 10^{-4}, with 10^5 time steps spent at each drive to allow the system to reach the steady state (the relaxation course). At the initial stage, all particles are distributed in the energy minima of the substrate potential. In this study, due to the periodic boundary conditions, we consider the system of size $100a \times 100a$. We use dimensionless system of units where the parameters $\mu = 0.2$, $f = 0.2$, $F_{ac} = 0.1$ and $a = 1$. It is noted that the interparticle equilibrium length a, not entering explicitly Eq.(3), appears only via the boundary condition, $x_{n+1}=x_1+Na$ and $y_{n+1}=y_1+Ma$ (N and M are intergers), to enforce a fixed density condition for the system. Based on the above-mentioned, we improved our MD fortran 90 code[20,21]

for the solution of Eq.(3). As the application of our code, the time averaged velocity <V> is numerically analyzed in the paper.

III. SIMULATION RESULTS

The time averaged velocity <V> as a function of external dc drive is presented for different angle α in Fig.2.

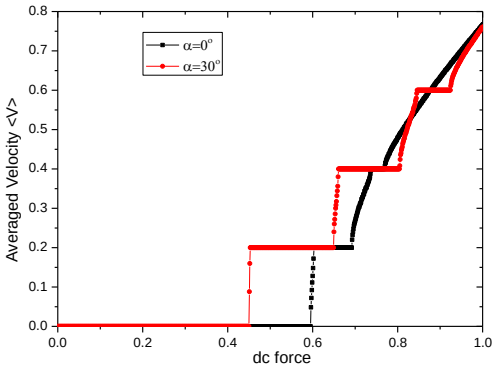

Figure 2. The averaged velocity<V> as a function of the dc force for the two different angles

As we can see from Fig.2, the curve for the average velocity as a function of the external dc force is characterized by the appearance of the staircase macroscopic response (called as Shapiro steps) for different angle α. The average velocities are in good with agreement with the resonant solution, i.e., the resonant velocities are given by $<V>=n\mu(n=0,1,2,3...)$. This ensures the reliability and accuracy of our fortran 90 code. It is noted that the system is driven by the periodic ac force, the two frequency scales are presented in the system: the frequency μ of the external ac force, and the characteristic frequency of the motion over the periodic triangular substrate potential driven by the dc force F_{dc}. The competition between the two frequency scales can result in the appearance of the staircases. The phenomena were also observed in the 1D FK model. Particularly, in the 2D Josephson junction arrays, the similar dependence has been obtained.

On the other hand, as we can see from Fig.2, the widths of steps are strongly influenced by the direction of dc force α. In the following paragraphs, we may gain an insight into the fundamental tribological concept, the static friction which is probably already encountered in some early stage during courses on classical mechanics or general physics and defined as the minimal threshold force needed to drive the relative motion. Particularly,

We mainly focus on the dependence of the critical depinning force on the different direction of the dc force α. By the way, the critical depinning force corresponds to the static frictional force in the fundamental tribology concept. In the numerical simulation, we have determined the static frictional force as the external dc force at which the system first has nonzero velocity.

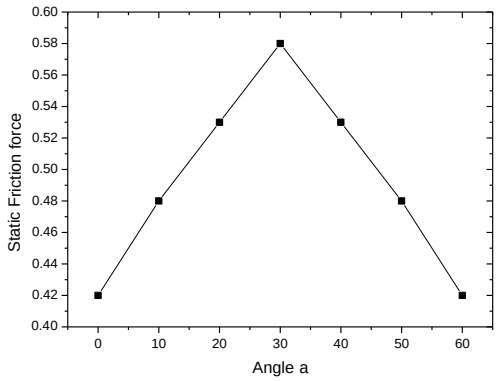

Figure3. The dependence of the static friction on the angle α

The dependence of the static frictional force Fs on the angle α are plotted in Fig.3. As clearly shown in Fig.3, variations of the direction of dc driven α will strongly affect the critical depinning force. Especially, the static frictional force is minimum value for $\alpha=0^0$ and 60^0. It are also noted that the curves are symmetric about $\alpha=30^0$. It is consequence of the symmetry of the system. We have also carried out more simulations for other parameter. All our simulation agrees with the regulation. In order to make the upper layer slide, all particles need to climb over the potential barrier of the other solid. Each particle will receive a resistance force in the opposite direction of the motion. Hence, in order to make all of atoms move together, the external driving force must be larger than the total sum of resistance force. This mechanism is one source of frictional force.

IV. CONCLUSION

In the manuscript, we have presented the numerical study of dynamical behavior of particles in the 2D triangular symmetric periodic substrate where these particles are driven by the dc and ac force. As an important application of our MD fortran 90 code, the staircase phenomena are observed in our simulations. The interesting feature the phenomena with increasing dc driven force is that the velocity <V> are given by the value sn $\mu(0,1,2,3...)$. Our results show that the direction of the dc driven force α plays a crucial role in the locked to sliding transition and the determination of the structure of the sliding state.

As a final statement, it is important to stress that the results could be of great importance for all real systems with particle motion which are driven by dc and periodic forces such CDW in solids and JJA that are motivated by fabrication of synchronization and superconducting devise.In these situations, these systems could be simplified by the Frenkel-Kontorova model. We hope that these results will simulate new works and experiments.

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