Numerical Study of Atom Interchange on Material Surface under Periodic Force

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Abstract—Nano-technology has developed to the level of direct control of single molecules and atoms. Recent experimental result with AFM has demonstrated the lateral atom interchange at room-temparature. In this paper, we discussed the modeling of two atom interchange on material surface with van der Waals force interaction. The numerical result show that coupled resonance can be the mechanism of the atom interchange phenomena.

1. Introduction

Since 1990s, experimental results have been reported on direct control of single molecules and atoms with use of scanning tunneling microscope (STM) and atomic force microscopy (AFM) [1, 2, 3, 4]. These experiments succeeded in positioning targeted single adatom to designated place on the material surface using sensing probe of STM or AFM. These processes have been also studied theoretically [5] and numerically [6]. In the continuation of this effort, recent experiment has succeeded in interchanging two adjacent adatoms on the surface by vibrating excitation of van der Waals force using AFM probe [4]. This success of atom interchange shows the possibility of direct control of nonconducting particles and building nano structure with mixture of different types of atoms and molecules on the surface. In this paper, we discuss the possibility of atom interchange between two different types of adatoms adjacent to each other on the material surface by the excitation of periodic external force. The surface and the adatoms interact each other with van der Waals (vdW) force and this vdW force is modeled by Lennard Jones (LJ) potential. In this model, two adatom particles are placed on the homogeneous material surface and they are trapped in the LJ potential field of the surface. The potential field of the surface is supposed to be identical on the two different adatoms, which means the nonlinear springs between the surface and each particles are same. Two adjacent adatoms also interact each other radially with LJ potential. In the discussion the resonant motion means the position interchange between the two particles or the break-out motion from the potential field which means the relative distance between the surface and a particle or the distance between the particles increase infinitely.

In this paper, we make a simple model to describe the atom interchange on the material surface and discuss the possibility of this resonant motion with the numerical simulation.

2. Two Particle Model Description

2.1. Model of Material Surface and Two Particles

Simplified model is studied to understand the dynamics of position interchange of two particles on the surface. As a simple model to describe two particle motion under the influence of potential field between the surface and the particles, the surface is modeled as y-axis and the position of two particles are given by the coordinates on the xy-plane to describe the distance from the surface and the distance between the particles. The configuration of the model is shown in Fig. 1.

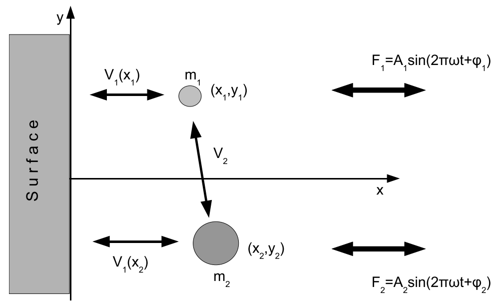

Figure 1: Two adatoms on material surface.

Here m_1 and m_2 are the masses of the two particles. x_1 and x_2 are the distance of two particles from the material surface and y_1 and y_2 are the y coordinates of two particles with respect to any choice of origin on the surface. It is assumed that the potential field by the surface is identical on both particles and the potential field between two particles is weaker than the potential by the surface. Since the LJ potential field has minimum point, two particle system has a equilibrium point which is invariant under the translation in y-direction. In the analysis, two particles undergo the oscillatory motion where the distance between the y-axis and particles and between particles are close to the equilibrium distances. The Hamiltonian can be written in the form:

$$H = \frac{(m_1\dot{x}_1)^2}{2m_1} + \frac{(m_1\dot{y}_1)^2}{2m_1} + \frac{(m_2\dot{x}_2)^2}{2m_2} + \frac{(m_2\dot{y}_2)^2}{2m_2} + V_1(x_1) + V_1(x_2) + V_2(r_{12}), \tag{1}$$

where $r_{12} = ((x_2 - x_1)^2 + (y_2 - y_1)^2)^{1/2}$.

The LJ potentials are given as follows:

$$V_1(x_1) = 4\epsilon_1 \left[\left(\frac{\sigma_1}{x_1}\right)^{12} - \left(\frac{\sigma_1}{x_1}\right)^{6} \right],$$

$$V_1(x_2) = 4\epsilon_1 \left[\left(\frac{\sigma_1}{x_2}\right)^{12} - \left(\frac{\sigma_1}{x_2}\right)^{6} \right],$$

$$V_2(r_{12}) = 4\epsilon_2 \left[\left(\frac{\sigma_2}{r_{12}}\right)^{12} - \left(\frac{\sigma_2}{r_{12}}\right)^{6} \right],$$

where ϵ_i, $i = 1, 2$, is the depth of the potential well and σ_i, $i = 1, 2$, is the collision diameter, the distance at which the potential is zero in each potential field. The distance at which $V_i = -\epsilon_i$ and the interparticle force becomes zero is $2^{1/6}\sigma_i$. The LJ potentials have the shape as shown in the Fig.2

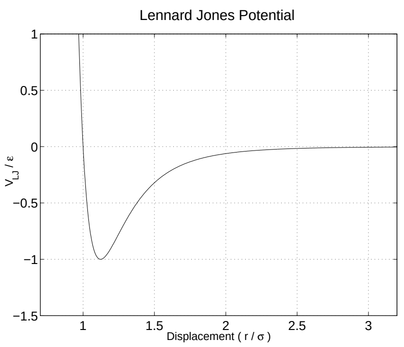

Figure 2: The schamatic graph of Lennard Jones potential

The dynamics of two particles is hamiltonian motion and its equation of motion can be written as the Hamilton's equation. Nondimensional variables can be introduced as follows:

$$q_1 = \frac{x_1}{\sigma_1},\ q_2 = \frac{y_1}{\sigma_1},\ q_3 = \frac{x_2}{\sigma_1},\ q_4 = \frac{y_2}{\sigma_1},$$

$$p_1 = \frac{\dot{x}_1}{\sigma_1},\ p_2 = \frac{\dot{y}_1}{\sigma_1},\ p_3 = \frac{\dot{x}_2}{\sigma_1},\ p_4 = \frac{\dot{y}_2}{\sigma_1}.$$

In these non-dimensional variables, the equation of motion becomes as follows:

$$\begin{cases} \dot{q}_1 = p_1,\ \dot{q}_2 = p_2,\ \dot{q}_3 = p_3,\ \dot{q}_4 = p_4, \\ \dot{p}_1 = \frac{4\epsilon_1}{m_1\sigma_1^2}(12q_1^{-13} - 6q_1^{-7}) \\ \quad + \frac{24\epsilon_2}{m_1\sigma_1^2}\left(\frac{\sigma_2}{\sigma_1}\right)^6 R^{-8}(q_1 - q_3)\left(2\left(\frac{\sigma_2}{\sigma_1}\right)^6 R^{-6} - 1\right) \\ \quad + A_1 \sin(2\pi\omega t + \phi_1), \\ \dot{p}_2 = \frac{24\epsilon_2}{m_1\sigma_1^2}\left(\frac{\sigma_2}{\sigma_1}\right)^6 R^{-8}(q_2 - q_4)\left(2\left(\frac{\sigma_2}{\sigma_1}\right)^6 R^{-6} - 1\right), \\ \dot{p}_3 = \frac{4\epsilon_1}{m_2\sigma_1^2}(12q_3^{-13} - 6q_3^{-7}) \\ \quad + \frac{24\epsilon_2}{m_2\sigma_1^2}\left(\frac{\sigma_2}{\sigma_1}\right)^6 R^{-8}(q_3 - q_1)\left(2\left(\frac{\sigma_2}{\sigma_1}\right)^6 R^{-6} - 1\right) \\ \quad + A_2 \sin(2\pi\omega t + \phi_2), \\ \dot{p}_4 = \frac{24\epsilon_2}{m_2\sigma_1^2}\left(\frac{\sigma_2}{\sigma_1}\right)^6 R^{-8}(q_4 - q_2)\left(2\left(\frac{\sigma_2}{\sigma_1}\right)^6 R^{-6} - 1\right), \end{cases} \tag{2}$$

where $R = ((q_3 - q_1)^2 + (q_4 - q_2)^2)^{1/2}$ and A_i, ω and ϕ_i are the non-dimensional amplitude and frequency and phase lag of the periodic excitation.

2.2. Small Oscillation near EP

The small oscillation analysis about the EP shows the existence of three nontrivial characteristic modes of the two particle motion and different characteristic frequencies correspond to each mode. To simplify the linear analysis, y-axis is replaced by a single fixed particle and the motion between one fixed particle and two free particles is studied. LJ potentials are replaced by the quadratic potentials of linear spring by the taylor expansion. The Taylor series for scalar valued function of multi variables has the following form:

$$\begin{aligned} T(x) &= H(X_0) + \nabla H(X_0)^T (X - X_0) \\ &\quad + \frac{1}{2}(X - X_0)^T \nabla^2 H(X_0)(X - X_0) + \cdots, \end{aligned} \tag{3}$$

where ∇H is gradient and $\nabla^2 H$ is Hessian. X_0 is 4-vector representing the equillibrium point and X is position vector. ∇H vanishes at X_0 and the small oscillation can be approximated with quadratic potential near the EP.

In the linear analysis, one characteristic frequency is zero and this frequency corresponds to the rotational symmetry of the free particle motion around the fixed particle. There are three positive eigenvalues in this linear system and they correspond to each characteristic mode.

3. Simulation of Atom Interchange

3.1. Parameter Setting

Parameters for numerical estimation is given in Table 1. The parameter values are arbitrarilly chosen in a reasonable range since the simulation is aimed for understanding on possible dynamics of simplified model.

Table 1: Parameter setting

Symbol	Value
ϵ_1	25×10^{-21} J
ϵ_2	15×10^{-21} J
σ_1	0.3 nm
σ_2	0.2 nm
m_1	2×10^{-10} kg
m_2	3×10^{-10} kg

3.2. Numerical Simulation

The numerical model is simulated with the variation of the frequencies and amplitudes of the periodic external force and the responsive motion of two particles is studied.

3.2.1. Free Oscillation

The free oscillation started from the initial position near the EP with zero velocity. In the simulation result, the x-directional frequency is observed to be about 40kHz and y-directional frequency is about 55kHz. The initial condition is set as follows:

$$q_1(0) = 1.1\,, q_2(0) = 0.35\,, q_3(0) = 1.1\,, q_4(0) = -0.35\,,$$

$$p_i(0) = 0\,, i = 1, 2, 3, 4\,,$$

The characteristic frequencies in the linear approximation near EP is in the range of 200kHz and this difference from that of direct observation of numerical simulation comes from that the LJ potential is not symmetric about the EP. Particles stay in the potential region outside of EP much longer time and in this region the paticle motion has low frequency.

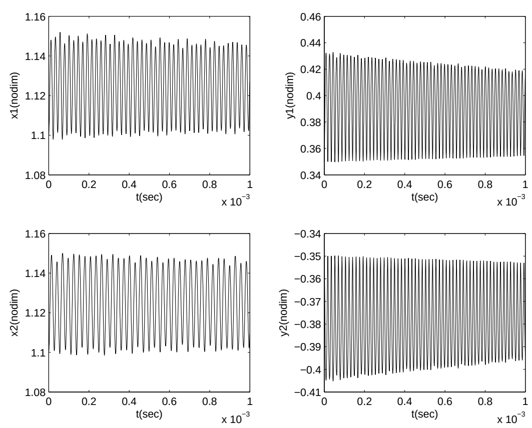

Figure 3: Free oscillations of two particles

3.2.2. Atom Interchange at Resonant Frequency

In the numerical simulation, the frequency of the external force is set at 30560Hz with $A_1 = 7.5 \times 10^8$, $A_2 = 5 \times 10^8$, $\phi_1 = 100$ and $\phi_2 = 0$ with the same initial condition as free oscillation. Here the external excitation is given only by x-directional force. In the setting of parameters given in the table 1, the atom interchange is observed as in Figure 4 and 5. Varing the frequency and amplitude of excitation, resonant frequency of the system is found to be about 30kHz. Here the x-directional excitation induced the resonance of the two particle system in y-directional oscillation and caused the energy transfer into the y-directional vibration via the coupled radial interaction. With the excitation of 30kHz periodic external force the amplitude needed for inducing the resonant motion is relatively small compared with that in different frequency range.

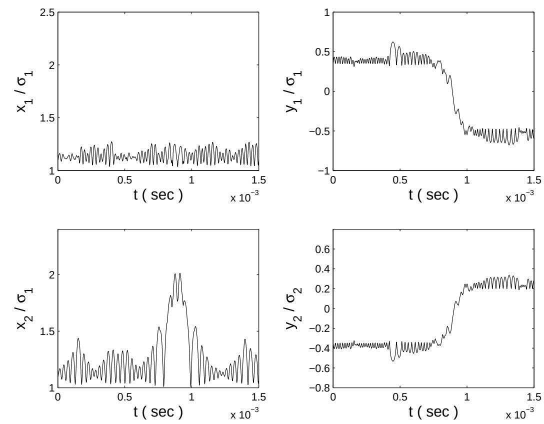

Figure 4: Atom interchange at 30kHz excitation

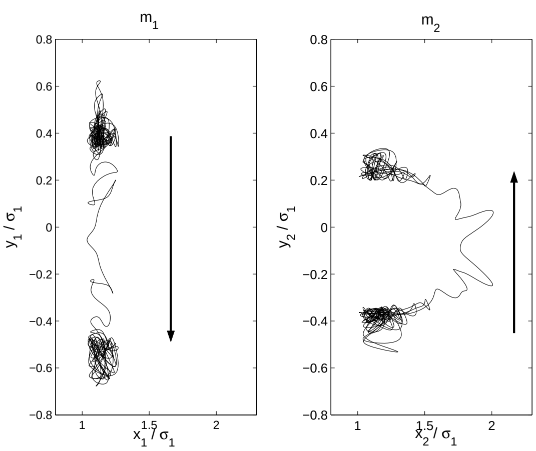

Figure 5: Trajectories of atom interchange

3.2.3. *Two Particle Motion at 200kHz Excitation*

Setting the excitation frequency as 200kHz which is in the normal operational frequency range of AFM, the required amplitude for resonant motion is about 50 to 100 times bigger than that of 30kHz. In the simulation the same amplitudes of excitation force as in 30kHz case are tested and this excitation doesn't cause the resont response of the particle motion and the responsive motion is very similar to free oscillation. When the amplitudes of excitation are increased to $A_1 = 4.5 \times 10^{10}$, $A_2 = 3 \times 10^{10}$, two particles show the resonant motion and one particle breaks out of the potential field of the surface.

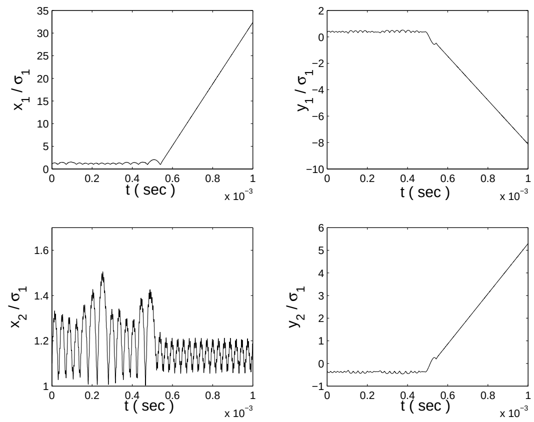

Figure 6: Particle motion at 200kHz excitation

3.3. Center of Mass Motion

The center of masses (CM) of two particle system shows y-directional momentum conservation under the periodic external force in x-direction. The x-coordinate of the CM shows oscillatory motion, but the y-coordinate of CM shows no change in time and keeps constant value even under the atom interchange or break-out motion of particles. This CM motion shows that the system keeps the y-directional momentum constant even when x-directional oscillatory motion induces y-directional oscillation in nonlinear coupled system of two particles and the energy in y-directional oscillation can increase.

4. Concluding Remarks

In this paper we discussed the simple model of the position interchange of adatoms on the material surface induced by the periodic external force in the form of vdW force. Numerical result shows the existence of the possible resonant frequency and its minimum excitation force for inducing resonant motion of the system. In the simple model of nonlinear coupled two particle system, we confirmed that x-directional excitation can cause y-directional resonant oscillation via the coupling radial interaction between two particles.

Controlability and separability of many particle system on material surface or in the liquid will be our future work. In the study of many particle system, dissipation of energy should be an important factor to be considered.

Acknowledgments

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