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Analysis of Cr Atoms Three-Dimensional Deposition Characteristics*

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Abstract

The semi-classical model is used to simulate the three-dimensional trajectory and deposition distribution of the chromium atoms in the Gaussian laser standing wave field using the Runge-Kutta method, and then the three-dimensional deposition stripes are also given, besides, the effects of atomic beam divergence, chromatic aberration and spherical aberration on deposition structure are also analyzed.

Keywords: Three-Dimensional Analysis, Atom Deposition, Cr Atoms, Gaussian Laser Standing Wave Field

1. Introduction

Nanotechnology is one of the fastest growing, most extensively studied, and putting up the most in the territory of science and technology currently, and it is known as the 21st-century science. Its purpose is to "research, develop and process those materials, devices and systems whose construction sizes are smaller than 100 nanometers in order to obtain the required functionality and performance [1]". This definition covers the process of nanofabrication, designs, characteristics and shapes of nanostructures, and measurement and characterization methods of nano-scale.

Nanometer measurement plays an irreplaceable important role in information collection and analysis of the nanotechnology. Nanometrology is involved with the intervals and displacements of the measurement objects within the range of 0.1 nm - 100 nm, the features of objects and their surface morphology, the development of technology and instrument of nano-micro-electronics, micro-machinery and precision measurement, the research on the interaction of probe and measured surface during nano-measurement as well as structures and intervention calibration methods of nano-devices. In order to achieve the calibration of nano-test-equipments in working sites or general laboratories, a good nano-scale length transfer standard is needed.

Therefore, to develop accurate and applicable nano-transfer standard is the present urgent problem and research priorities. Its technical routes are mainly along three directions, and one of it is laser focused atomic deposition for Nanometer-scale structure. In NIST, McClelland *et al.* once obtained one-dimensional optical gratings of chromium using laser focused atomic deposition technique, the uncertainty of average pitch of focused atomic deposition process manufacturing standard sample was 0.0049 nm [2]. In February 1998, the average pitch of Cr sample which was fabricated by NIST and deposited on Sapphire was 212.7787 ± 0.0049 nm (The substrate temperature was 29˚C) [3]. And then in 2002, the average pitch measured by optical diffraction was confirmed to be 212.7777 ± 0.0069 nm [4]. This was in good line with the expected pitch 212.7705 ± 0.0049 nm at 22˚C [4]. The uncertainty of this average pitch was 10^{-5}, which can be directly traced to the absolute atomic transition frequency. Therefore, the produced nano-grating structures are very accurate, and are accordance with the requirements of nano-transfer standard.

The basic principle of laser focused atomic deposition for nanostructure is that uses radiation pressure of resonant laser standing wave field to make density of atoms' high-collimated beam to generate periodic distribution in space, and then these neutral atoms are deposited on a substrate to form nano-scale grating structures. **Figure 1** shows the schematic of laser focused atomic deposition for nano-grating structure.

For theoretical analysis of the laser focused atomic deposition for nano-grating, some research teams both at home and abroad have done one-dimensional and two-dimensional simulations for different neutral atoms, and

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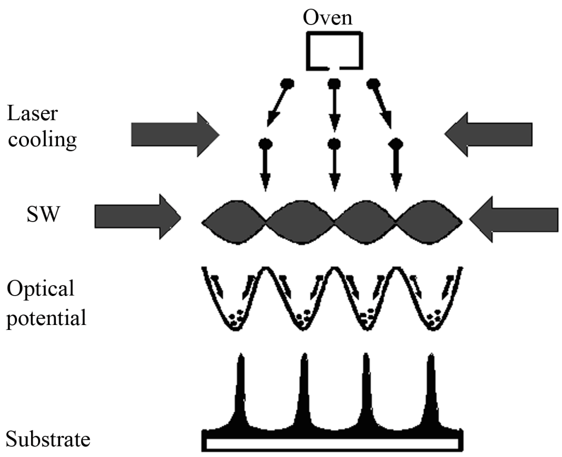


Figure 1. Principle of laser focused Cr atomic deposition nano-grating structure.

have achieved numerous of significance results for the practical application, but the three-dimensional analysis of the research has not been reported yet. In this paper three-dimensional trajectory model of Cr atoms in the Gaussian standing wave laser field is built and a single-atom three-dimensional trajectory simulation algorithm is induced. In the basis of single-atom three-dimensional trajectory algorithm, semi-classical theory is used to analyze three-dimensional trajectory of Cr atoms under the action of dipole force and explore motion characteristics of atoms in laser standing wave field. At last, influence of some factors such as spherical aberration, chromatic aberration, atomic beam divergence on the process of nano-grating is also analyzed based on the three-dimensional trajectories of neutral atoms.

2. Three-Dimensional Trajectory Calculation Models of Cr Atoms

In the laser standing wave field, intensity of laser field changes according to $I \propto \sin^2(kx)$ along the direction of wave vector ***k***. For the Gaussian standing wave laser field, assuming that its distribution is along the x direction, and its waist radius along the y and z directions are both ω_0, so its intensity can be expressed as:

$$I(x,y,z) = I_{\max} e^{\left(-2z^2-2y^2\right)/w_0^2} \sin^2(kx) \tag{1}$$

Here $I_{\max}$ is the maximum intensity of the standing wave field. When the system reaches a steady state, the steady-state dipole potential of laser standing wave field can be described by:

$$U(x,y,z) = \frac{\hbar\delta}{2}\ln\left[1+p(x,y,z)\right] \tag{2}$$

where $p(x,y,z) = \dfrac{I(x,y,z)}{I_s}\dfrac{\Gamma^2}{\Gamma^2+4\delta^2} = p_o G(x,y,z)$,

$$p_o = \frac{I_o}{I_s}\frac{\Gamma^2}{\Gamma^2+4\delta^2},$$

and that Γ and I_s are respectively natural linewidth and saturation intensity of atom. Therefore, the motion equation of atoms in the Gaussian standing wave laser field can be expressed as:

$$\begin{cases} \ddot{x} + \dfrac{1}{m}\dfrac{\partial U(x,y,z)}{\partial x} = 0 \\ \ddot{y} + \dfrac{1}{m}\dfrac{\partial U(x,y,z)}{\partial y} = 0 \\ \ddot{z} + \dfrac{1}{m}\dfrac{\partial U(x,y,z)}{\partial z} = 0 \end{cases} \tag{3}$$

Here $\dot{x}$ 、 $\dot{y}$ 、 $\dot{z}$ represent the atomic velocity along three directions respectively. So we can get:

$$\begin{cases} x''\dot{z}^2 + x'\ddot{z} + \dfrac{1}{m}\dfrac{\partial U(x,y,z)}{\partial x} = 0 \\ y''\dot{z}^2 + y'\ddot{z} + \dfrac{1}{m}\dfrac{\partial U(x,y,z)}{\partial y} = 0 \end{cases} \tag{4}$$

Then under the action of conservative dipole force, total energy of atom can be represented by:

$$E_o = T + U = \frac{1}{2}m\left(\dot{x}^2+\dot{y}^2+\dot{z}^2\right) + U(x,y,z) \tag{5}$$

And because

$$\begin{cases} \dot{x} = \dfrac{\mathrm{d}x}{\mathrm{d}t} = \dfrac{\mathrm{d}x}{\mathrm{d}z}\dfrac{\mathrm{d}z}{\mathrm{d}t} = x'\dot{z} \\ \dot{y} = \dfrac{\mathrm{d}y}{\mathrm{d}t} = \dfrac{\mathrm{d}y}{\mathrm{d}z}\dfrac{\mathrm{d}z}{\mathrm{d}t} = y'\dot{z} \end{cases} \tag{6}$$

Here x' and y' are respectively differential of x to z and y to z.

Finally, according to the Equations (3)-(6), three-dimensional trajectory equation of Cr atoms can be obtained:

$$\begin{cases} x''\dfrac{2(E_o-U)}{m\left(1+x'^2+y'^2\right)} + x'\left(-\dfrac{1}{m}\dfrac{\partial U}{\partial z}\right) + \dfrac{1}{m}\dfrac{\partial U}{\partial x} = 0 \\ y''\dfrac{2(E_o-U)}{m\left(1+x'^2+y'^2\right)} + y'\left(-\dfrac{1}{m}\dfrac{\partial U}{\partial z}\right) + \dfrac{1}{m}\dfrac{\partial U}{\partial y} = 0 \end{cases} \tag{7}$$

Making use of numerical algorithm, Equation (7) is solved by setting adapted step fourth-order Runge-Kutta algorithm, and three-dimensional deposition characteristics of Cr atoms in the Gaussian standing wave laser field are also studied.

3. Simulation Results and Analysis

In this paper, waist radius of Gaussian laser beam is set to be $\omega_0 = 100\ \mu m$, and parameters of Cr atoms in laser standing wave field corresponding to ${}^7S_3 \rightarrow {}^7P_4^0$ transition spectral line are respectively: transition wavelength $\lambda = 425.55$ nm, natural linewidth $\Gamma = 5$ MHZ, saturation intensity $I_s = 85\ \mathrm{W/m^2}$ and detuning $\delta = +200$ MHZ. When δ is far greater than Γ, in order to make the Cr atoms be focused to positions where the light intensity is strongest through the role of the optical potential well, laser power needed is [5]:

$$P_{\text{focus}} = 5.37\frac{\pi E_k I_s \delta}{\hbar \Gamma k^2}.$$

For the longitudinal velocity $T_0 = 1900$ K, its most probable velocity is $V_Z = 955\ \mathrm{m/s}$, and at this time focused power of Cr thermal atomic beam is $P_{\text{focus}} = 3.93$ mW [6].

Figure 2 shows the normalized intensity distribution of Gaussian standing wave laser field. It can be seen that the distance between two nodes (antinodes) of standing wave field is half the wavelength. From this we can see that when using atom laser standing wave field to focus the atoms, the obtained nano-stripe spacing is also half the laser wavelength. Thus the standing wave field is similar to "atomic lens" with atom-focus feature, and imaging, focusing behaviors of the "lens" depend on the characteristics of manipulated atoms. Therefore, the final distribution of atomic beam can be adjusted by adjusting light field intensity, light field distribution, light field size and other parameters [7].

Figure 3 shows the trajectory of a single atom. The atom with an initial speed $V_Z = 955\ \mathrm{m/s}$ enters into the standing wave along the z direction, and its motion trajectory will change under the effect of dipole force. Three-dimensional trajectory of Cr atoms in laser standing wave field is shown in **Figure 4**. From **Figure 4** it can be seen that under ideal conditions, Cr atoms are focused to the center of the standing wave field under the action of potential trap.

Considering the role of y direction, **Figure 5** shows the deposition three-dimensional stripes structure of chromium atoms under ideal conditions in the Gaussian standing wave laser field conditions. It can be seen from the **Figure 5** that under the action of Gaussian standing wave field, the half-wavelength periodic stripes are formed along the x direction, and the height of the stripes will gradually reduce starting from the center along the y direction, besides, its full width at half maximum (FWHM) will be on the increase, that is to say, the quality of the deposition stripes will become worse along they direction from the center to both sides.

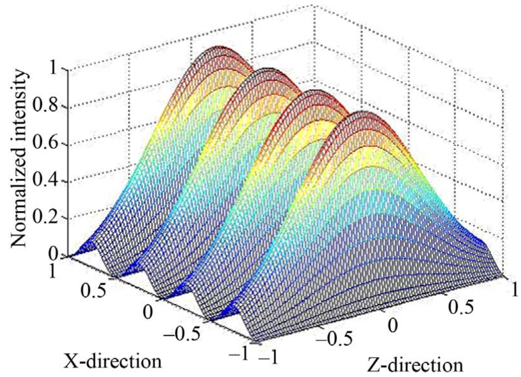


Figure 2. Normalized intensity of Gaussian laser standing wave field.

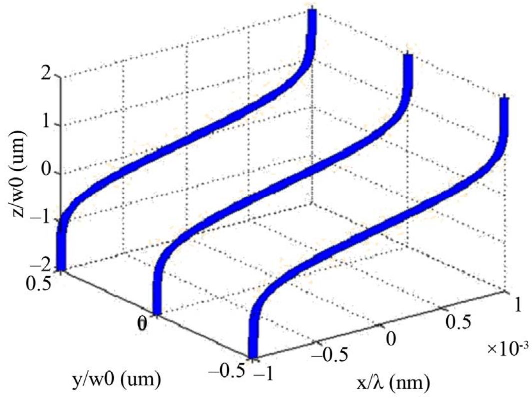


Figure 3. Trajectories of single Cr atom.

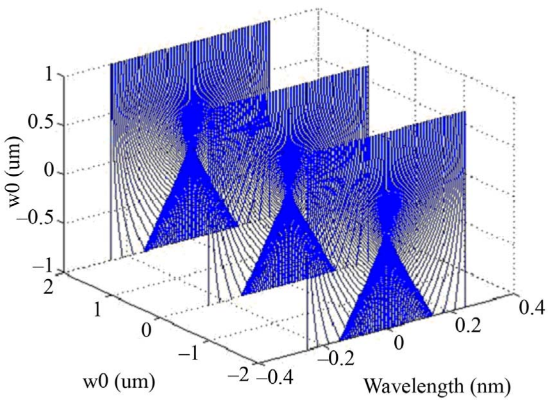


Figure 4. Trajectories of Cr atoms.

However, in real conditions, the deposition of chromium atoms is influenced by many factors, which will affect the final results of the deposition. The role of the laser standing wave field can be assimilated to a lens, so these factors can be described by aberrations in the field of optics including atomic beam divergence, chromatic aberration and spherical aberration.

For thermal atomic beam, it also has some transverse velocity, which satisfies the Gaussian distribution [8],

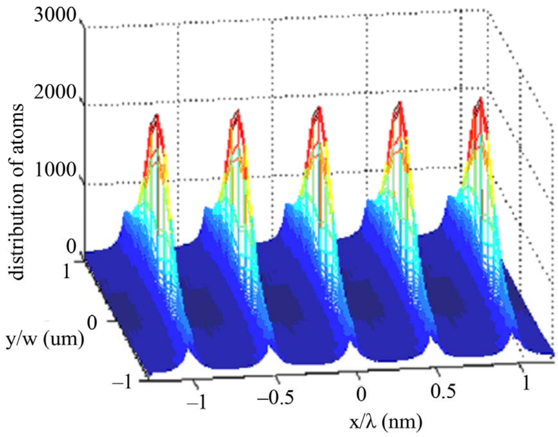


Figure 5. Three dimensional stripes of Cr atom under ideal conditions.

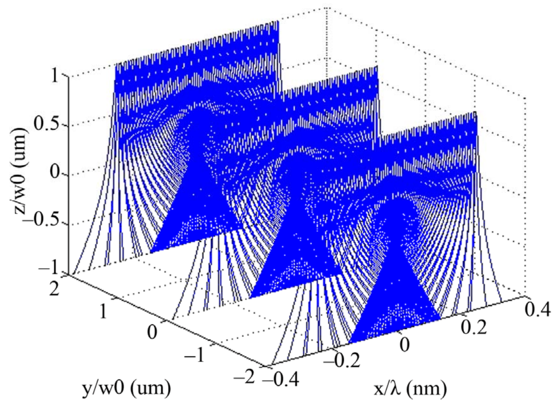


Figure 6. Trajectories of chromium atoms under the influence of atomic beam divergence.

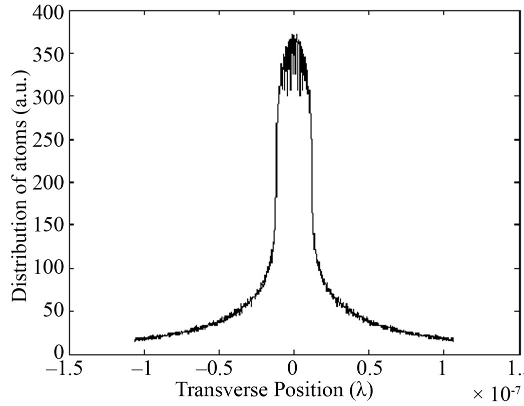
corresponding to a certain divergence angle. Although the divergence angle will be reduced after laser cooling,it is impossible to be reduced to zero, so there is always a certain amount of transverse velocity and divergence angle distribution for the incident atom beam in standing wave. **Figure 6** shows the atomic trajectory affected by atomic beam divergence.

Figure 7 is the deposition distribution and three-dimensional stripes structure of chromium atoms under the influence of atomic beam divergence. From the figure we can see that the atomic beam divergence has led to widen the atomic deposition stripes. This is because the transverse vibration cycle of the atoms has been changed by initial velocity V_x. Comparing with the ideal deposition, many atoms are deposited around the minimum potential field, which results in a certain width with the grating structure.

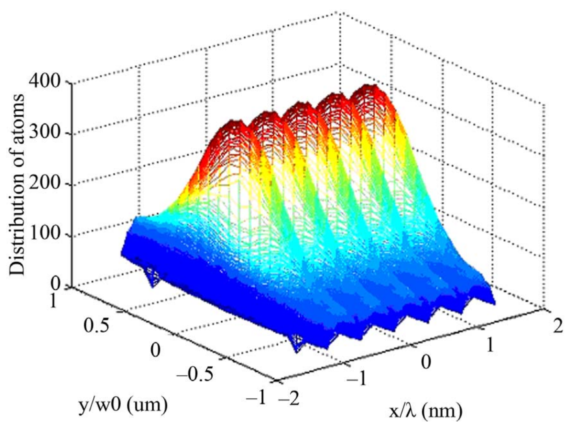
As the real atomic beam is not monoenergetic atomic beam, there is a longitudinal velocity distribution to atomic beam, which obeys Maxwell-Boltzman distribution [9]. After standing wave lens focusing, the parallel incident atoms with different speed are not intersected to the same point, but in a region, that is to say, there will be a range of change to focal length, which corresponds to chromatic aberration in particle optics. The atomic trajectory deviation caused by longitudinal velocity can be expressed as [8]:

$$\delta x = -2\,\varphi a \frac{\mathrm{d}f}{\mathrm{d}a}\frac{\delta V_z}{V_z}$$

Figure 8 shows atomic trajectories under the influence of chromatic aberration, from which we can see there is a range of change to focal length for the parallel incident atoms with different longitudinal velocity the component after entering into the standing wave field. **Figure 9** is the deposition distribution and three-dimensional stripes structure of chromium atoms under the influence of



(a)



(b)

Figure 7. (a) Deposition distribution of chromium atoms under the influence of atomic beam divergence; (b) Three dimensional stripes of chromium atoms under the influence of atomic beam divergence.

chromatic aberration. It can be seen from the figure there is a broadening to deposition stripes of chromium atoms under the influence of chromatic aberration. At this time full width at half maximum (FWHM) and contrast of

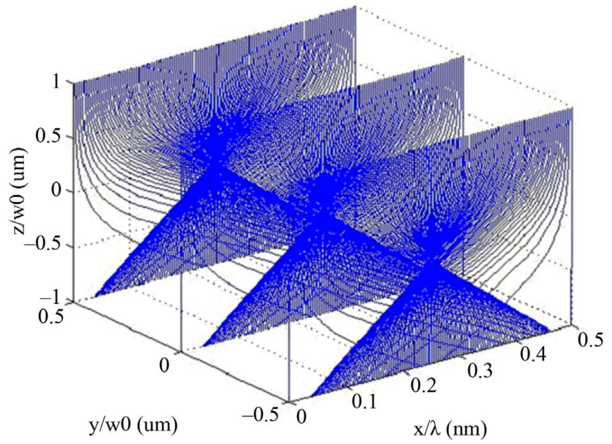


Figure 8. Trajectories of chromium atoms under the influence of chromatic aberration.

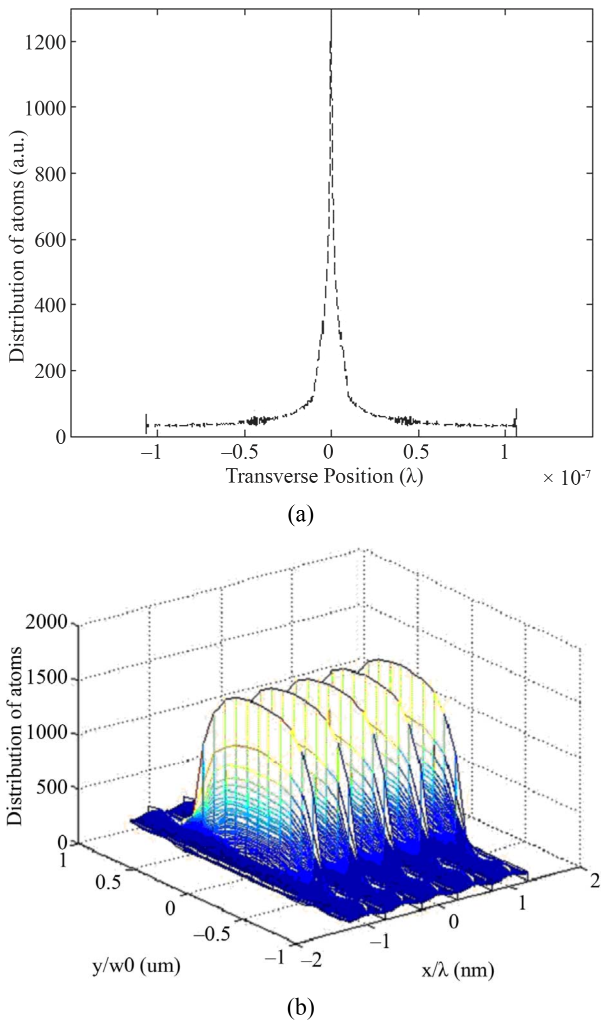


Figure 9. (a) Deposition distribution of chromium atoms under the influence of chromatic aberration; (b) Three dimensional stripes of chromium atoms under the influence of chromatic aberration.

chromium atoms obtained are respectively about 1.4 nm and 40 by using cumulative method.

Spherical aberration results from the higher order terms of motion equations, which leads to the actual trajectories of atoms deviating from trajectories obtained by the paraxial equation. The traditional method to estimated spherical aberration is to expand motion equations and deal with their high-order terms as a perturbation of paraxial equation. Here, the impact of spherical aberration atomic beam imaging can be seen from the numerical solution of motion equations of atoms in the standing wave field.

Figure 10 shows atomic trajectories under the influence of spherical aberration. At first, the atoms move parallel to the z-axis at the most probable initial velocity, then intersect different locations after entering into the laser standing field. Due to different incident locations, spherical aberration is generated, ultimately making the deposition of deposition spot diffusion which causes the resulting widen deposition stripes. **Figure 11** is the deposition distribution and three-dimensional stripes structure of chromium atoms under the influence of spherical aberration. Through the numerical solution of the motion equations, observing the impact of spherical aberration on deposition structure is direct and accurate, and its deficiency is not provided simple expression describing full width at half maximum (FWHM).

4. Conclusions

In summary, the three-dimensional trajectory of chromium atoms is simulated by using four-order Runge-Kutta arithmetic. Based on the discussion of reaction with laser standing wave, the motion characteristics of chromium atom are analyzed and the three dimensional

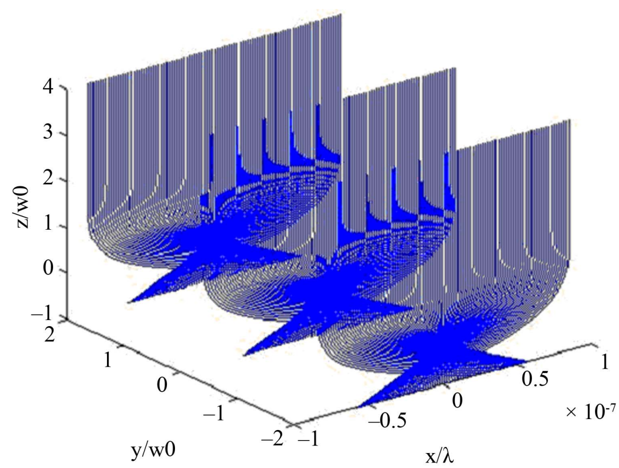
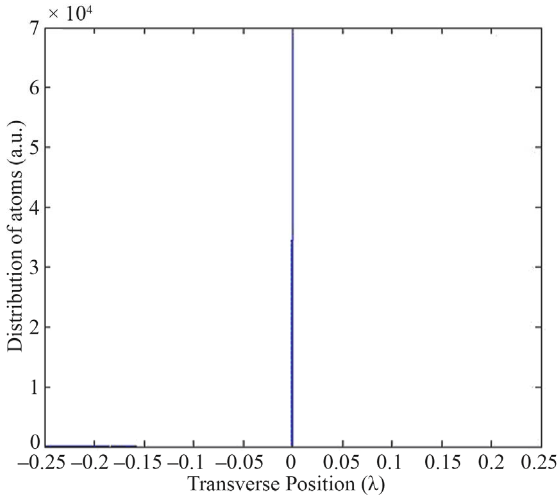
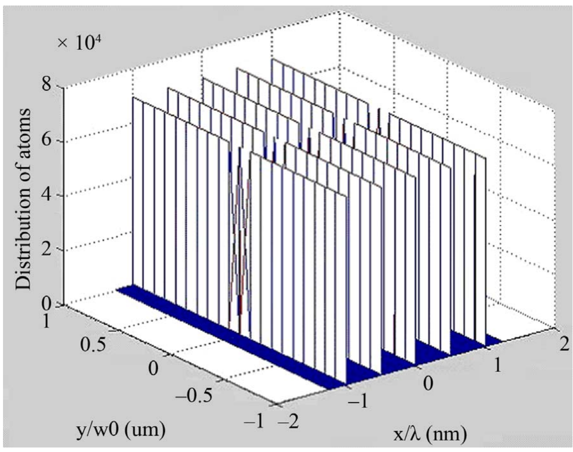


Figure 10. Trajectories of chromium atoms under the influence of spherical aberration.



(a)



(b)

Figure 11. (a) Deposition distribution of chromium atoms under the influence of spherical aberration; (b) Three dimensional stripes of chromium atoms under the influence of spherical aberration.

stripe structure is also simulated. From the simulation we can see that the atoms can be focused, and the periods of the stripe is equal to half wavelength. What's more, the transverse velocity, chromatic aberration and spherical aberration of atoms will affect the characteristics of the stripe.

5. References

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