

Effects of divergence angle on deposition of neutral atoms

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Abstract: Using neutral chromium atoms for the fabrication of nanometer-scale ordered structures is a new method of generating nanostructures on a substrate. But all the information of nano-gratings deposited by laser standing wave field can not be given only through one-dimensional or two-dimensional analysis. Three-dimensional analysis of the effects of atomic beam divergence angle on the process of fabricating nano-grating was discussed based on the three-dimensional motion model of Cr atoms in Gaussian standing wave laser field. The study shows that the preparation of a high-collimated and transversely cooled atomic beam, typically under 0.6 mrad, is essential to minimize the severely disadvantageous effects for deposition of atoms in laser standing wave.

Key words: three-dimensional analysis; neutral atom lithography; divergence angle; Gaussian laser standing wave field

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发散角对中性原子沉积特性的影响

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摘要: 利用激光驻波场操纵中性原子沉积纳米光栅结构是一种新颖的制备纳米计量标准技术, 但采用传统的一维和二维方式对激光驻波场操纵中性原子沉积过程的分析缺乏纳米光栅的全貌信息, 而采用三维分析方法则能给出纳米光栅的三维全貌信息, 对结果的分析越精确。针对此, 基于采用三维分析方法建立了激光驻波场与中性原子作用的模型, 通过三维分析实现了不同原子束发散角条件下中性原子运动轨迹及沉积结果的三维仿真, 结果显示当中性原子束发散角小于 0.6 mrad 时, 所获得的纳米光栅的沉积质量较好, 而超过 0.6 mrad 后所沉积的纳米光栅将会出现分裂现象。

关键词: 三维分析; 中性原子; 发散角; 高斯激光驻波场

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0 Introduction

The fabrication of nano-scale structures by neutral atom lithography has the potential to significantly put forward the nanotechnology [1]. In comparison with similar traditional technologies, this neutral atom lithography has a number of potential advantages. Due to the extremely small de Broglie wavelength, the resolution can be in principle very high. Further more, the direct-write process effectively prevents any damage to the substrate, also any chemical reaction. Because they are charge-neutral, unlike electrons or ions, neutral atoms are not affected by the space charge effect that can make it very difficult to concentrate many particles into a very small region. It could be a vital technology to extend the device miniaturization and nano-metrology [2-4].

Since the purpose of atom lithography is to deposit small features, and there are some effects that contribute to broadening of the features, such as divergence angle of atomic beam, distribution of longitudinal velocity of atoms and spherical aberration. The structure width deteriorates fast with the increase of the atomic beam divergence angle, and the SW optical potential is extremely shallow and the atomic velocities along the SW direction must be low for the atoms to be "trapped" in SW nodes(antinodes) [5-6]. For these two reasons, the divergence angle of atomic beam has very strong effect on the nanometer scale features. For theoretical analysis of neutral atom lithography for nano-grating structure, some research teams both at home and abroad have done one-dimensional and two-dimensional simulation for different neutral atoms, and 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, taking neutral chromium atoms as working particle, three-dimensional analysis of the effects of atom beam divergence angle on the process of fabricating nano-

grating is discussed based on the three-dimensional motion model of Cr atoms in Gaussian standing wave laser field.

1 Three-dimensional motion model of Cr atoms in Gaussian standing wave laser field

In the Gaussian standing wave laser 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 [7]:

$$I(x,y,z) = I_{\max} e^{(-2z^2 - 2y^2)/\omega_0^2} \sin^2(kx) \quad (1)$$

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 [8]:

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

Where $p(x,y,z) = \frac{I(x,y,z)}{I_s} \frac{\Gamma^2}{\Gamma^2 + 4\delta^2} = p_0 G(x,y,z)$, $p_0 = \frac{I_0}{I_s} \frac{\Gamma^2}{\Gamma^2 + 4\delta^2}$, and that Γ and I_s are respectively natural line width and saturation intensity of atom [9]. Therefore, the motion equation of atoms in the Gaussian standing wave laser field can be expressed as:

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

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

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

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

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

And because:

$$\begin{cases} \dot{x}=\frac{dx}{dt}=\frac{dx}{dz}\frac{dz}{dt}=x'z' \\ \dot{y}=\frac{dy}{dt}=\frac{dy}{dz}\frac{dz}{dt}=y'z' \end{cases} \quad (6)$$

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

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

$$\begin{cases} x''\frac{2(E_o-U)}{m(1+x'^2+y'^2)}+x'\left(-\frac{1}{m}\frac{dU}{dz}\right)+\frac{1}{m}\frac{dU}{dx}=0 \\ y''\frac{2(E_o-U)}{m(1+x'^2+y'^2)}+y'\left(-\frac{1}{m}\frac{dU}{dz}\right)+\frac{1}{m}\frac{dU}{dy}=0 \end{cases} \quad (7)$$

Making use of numerical algorithm, Eq. (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 is also studied.

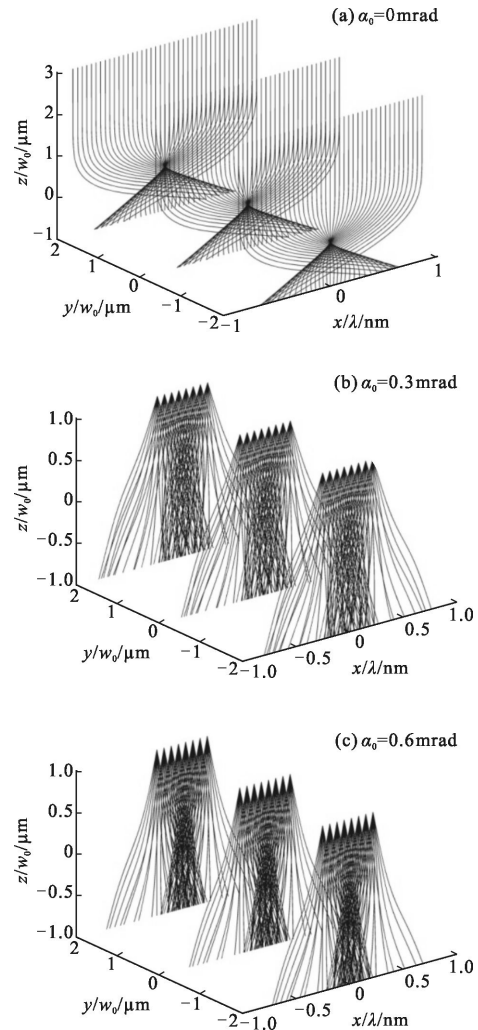
2 Simulation results and analysis

There are two different types of inter-action forces that can be used to manipulate neutral chromium atoms^[10], and only the dipole force can be used to focus the atoms. In the case of large detuning, the dipole force is proportional to the intensity of electromagnetic field at the position of the neutral atom^[9]. Depending on the detuning of the laser frequency with respect to the resonance frequency, the neutral chromium atom feels a force towards high or low intensity regions. For neutral chromium atoms, the standing wave field acts like an array of cylindrical lenses and can focus them onto the substrate and then form nanometer structure^[12].

In this paper, waist radius of Gaussian laser beam is set to be $\omega_0=100 \mu\text{m}$, and parameters of Cr atoms in laser standing wave field corresponding to ${}^7\text{S}_3 \rightarrow {}^7\text{P}_4^0$ transition spectral line are respectively: transition wavelength $\lambda=425.55 \text{ nm}$ natural line width $\Gamma=5 \text{ MHz}$, saturation intensity $I_s=85 \text{ W/m}^2$ and detuning $\delta=+200 \text{ MHz}$. 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: $P_{\text{focus}}=5.37\frac{\pi E_s I_s \delta}{\hbar \Gamma k^2}$. For the longitudinal velocity $T_0=1900 \text{ K}$, its most probable velocity is $V_z=995 \text{ m/s}$, and at this time focused power of Cr thermal atomic beam is $P_{\text{focus}}=3.93 \text{ mW}$.

For thermal atomic beam, it has some transverse velocity, which satisfies the Gaussian distribution, corresponding to a certain divergence angle. Figure 1 shows the three-dimensional atomic trajectories of chromium atoms affected by different atomic beam divergence angle α_0 . In Figure 1 (a), $\alpha_0=0 \text{ mrad}$, that is to say, the atomic beam has no transverse velocity component. The atomic beam divergence angles are respectively 0.3 mrad , 0.6 mrad , 1 mrad in Figure 1(b),



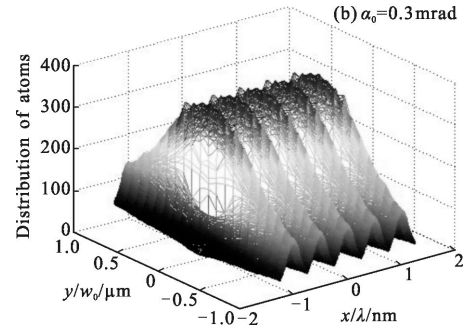
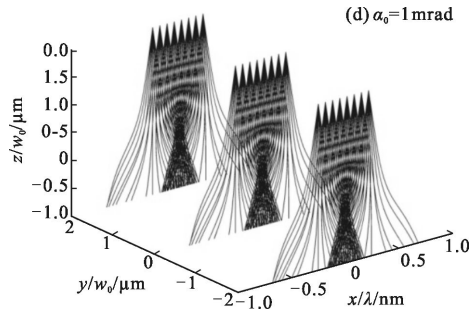


Fig.1 Three-dimensional trajectories of Cr atoms affected by atomic beam divergence angle

(c) and (d). From Fig.1, it can be seen that the deposition region becomes wider with the increase of atomic beam divergence angle.

The full width at half minimum (FWHM) is a simple and well defined number, which can be used to compare the quality of the nanometer deposition. From Fig.3, it can be seen that when the divergence angle equals 0 mrad, the FWHM of the deposition stripe is 2.75 nm, when the divergence angle of the atomic beam increases to 0.3 mrad, the FWHM of the deposition stripe is 26.52 nm. When the divergence angle is 0.6 mrad, the FWHM equals 48.35 nm and the FWHM is 137.86 nm when the divergence angle equals 1.0 mrad.

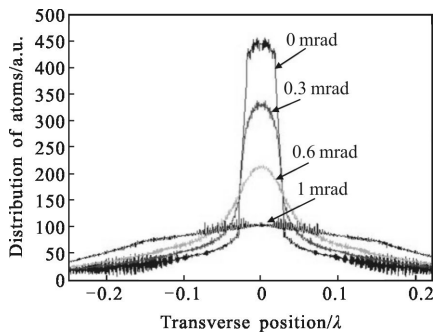
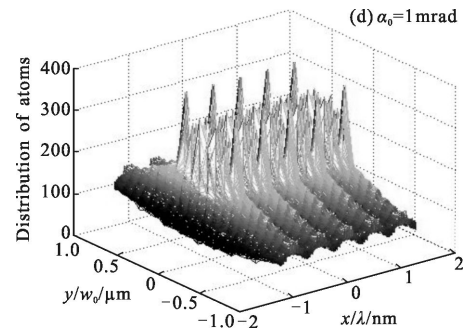
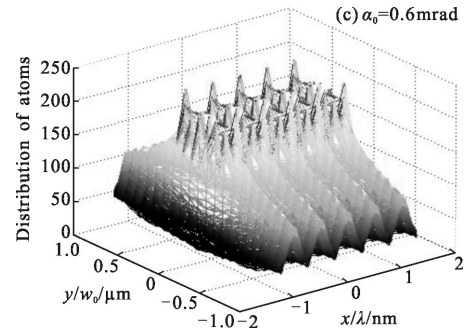


Fig.3 Three-dimensional of stripes of Cr atoms affected by atomic beam divergence angle

Fig.2 Deposition distribution of Cr atoms affected by atomic beam divergence angle

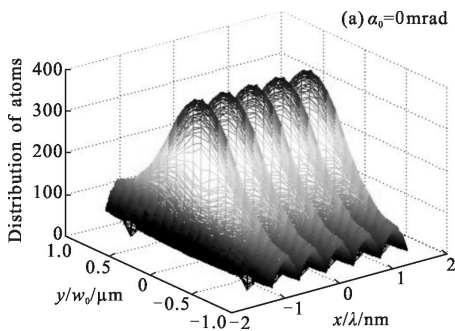


Figure 2 and Figure 3 are the deposition distribution and three-dimensional stripes structures of chromium atoms under the influence of atomic beam divergence. It can be seen that the atomic beam divergence has led to widening of the atomic deposition stripes and the heights of deposition stripes become lower with the increase of atomic beam divergence angle. This is because the transverse vibration cycle of the atoms has been changed by initial velocity V_x . Compared with the ideal deposition, many atoms are deposited around the minimum potential field, which results in a certain width with the grating structure. So in order to get high quality nanometer structure by neutral atom lithography, the divergence of atomic beam must be

compressed to some extent.

3 Conclusion

Atomic beam spreading plays an important role in determining the deposition nanometer quality, so the preparation of a high-collimated and transversely cooled atomic beam, typically under 0.6 mrad, is essential to minimize the severely disadvantageous effects for deposition of atoms in laser standing wave.

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