



## Full Paper

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## 3-D analysis of characteristics in fundamental mode Gaussian laser standing wave with straight edge diffraction

### Abstract

Based on scalar optical theory, the fundamental mode Gaussian laser standing wave model is built with Fresnel straight edge diffraction effect in the process of laser-focused Cr atoms. By numerical analysis and 3-D simulation on optical potential, characteristics in the laser standing wave are described under the influence of the distances from diffraction edge to mirror and laser medial axis to substrate surface, respectively. The results show that diffractive degree of the laser field will be changed for the substrate placement, and the structure of optical potential will be achieved optimal when the distance from diffraction edge to mirror equals 0.51 cm.

### Key Words

Fundamental mode Gaussian laser; Straight edge diffraction; 3-D simulation.

## INTRODUCTION

The converging technology that neutral atoms are manipulated by laser standing wave, as one of the important branches in atom lithography, has given rise to considerable attention over the past 25 years<sup>[1,2]</sup>. The stable structure of chromium grating can be successfully used as a nanoscale length benchmark using the deposition technique of laser focusing<sup>[3]</sup>. During the interaction between laser standing wave field and neutral atoms, Cr atomic beams, which are collimated by laser cooling, will be converged on the peaks or valleys under operation of the dipole force. And then the fabrication of 2-D nano-patterns will be accomplished after depositing it on the substrate<sup>[4]</sup>. However, the edge of the substrate, just as a semi-infinite diffraction screen of opaqueness, which obstructs some laser propagations in the practical deposition experiment. Consequently, a physical model based on Fresnel straight edge diffraction is constituted between the substrate edge and laser beams<sup>[5]</sup>. In 2009, F. Tantussi and V. Mangasuli controlled cesium scale by using the converging technology, and they certified that spatial distribution of the de-

posited atoms is partially modulated according to the standing wave periodicity, shape and direction<sup>[6]</sup>. In 2011, Nikolai Korneev employed the interferometer to optical testing with a straight edge while substrate was located at the central point of laser beams, the interferograms of which were evaluated for the optical quality<sup>[7]</sup>. In 2012, taking 1-D Cr atomic deposition as an example, Wang Jianbo presented an experiment method, which precisely defined the position of standing wave relative to deposition substrate<sup>[8]</sup>. The same year, Zhang Baowu and Ma Yan simulated to the light intensity of Gaussian laser in straight edge diffraction field, in addition, they explained the formative substance of laser standing wave deeply<sup>[9]</sup>. For diffraction theory, in 2008, Yusuf Z. Umul separated the physical optics surface integral into two sub-integrals which represented the reflected and diffracted fields, and the potential function of the boundary diffraction wave theory was deduced using the same forms, resulting in the relation between the physical optics and boundary diffraction wave theory<sup>[10]</sup>. In 2012, Kazi Monowar Abedin and S. M. Mujibur Rahman applied the iterative Fresnel integrals method for the numerical computation of Fresnel

diffraction, and simulated to light intensity of the actual diffraction patterns<sup>[11]</sup>. But, the approximate approach must be made, for which Fresnel straight edge diffraction usually does not have accurate analytic solution<sup>[12]</sup>.

In this paper, a fundamental mode Gaussian laser standing wave is established based on an approximation theory about the Fresnel straight edge diffraction. Then through 3-D simulation to the optical potential in laser standing wave, we discuss the impact on the position where substrate is placed. It provides a basic theoretical foundation and data information for the experimental research on atom lithography<sup>[13]</sup>.

## MODEL BUILDING

In the schematic diagram, Gaussian laser beams propagate along the  $x$  direction while collimated Cr atomic beams move along the  $z$  direction. The origin coordinate  $O$  is set on the laser beam waist center position, as well as the mirror  $M$ . Coordinate system  $z_1P_1y_1$  is the place where the diffraction screen is built, that is, the position of substrate edge. Coordinate system  $zPy$  is defined as the observation screen, the location of which is selected between diffraction screen and mirror (Figure 1).

According to coordinates mentioned above, when

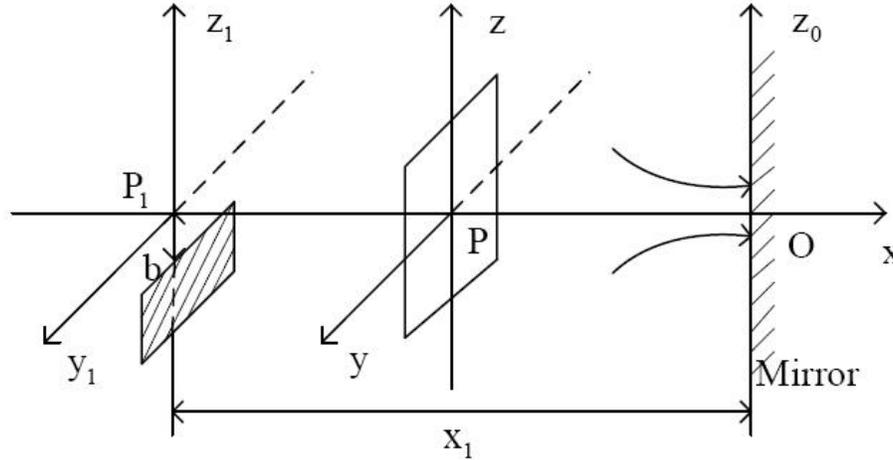


Figure 1 : The basic principle model of Fresnel straight edge diffraction. This diagram shows the formation of standing wave using Gaussian laser. The substrate edge stops a part of laser beams, then diffraction wave goes back along the same route when it comes across mirror, and finally, standing wave field is shaped on the observation screen, which composites the incident wave with reflected wave.

incident Gaussian laser goes through a light transmission aperture  $\Sigma$ , the Fresnel diffraction distribution of complex amplitude on observation screen can be expressed<sup>[14]</sup>.

$$\tilde{E}_1(x, y, z) = \frac{\exp(ikd)}{i\lambda d} \iint_{\Sigma} \tilde{E}_1(x_1, y_1, z_1) \exp\left\{\frac{ik}{2d}[(y - y_1)^2 + (z - z_1)^2]\right\} dy_1 dz_1 \quad (1)$$

Where  $\lambda$ ,  $k$ ,  $x_1$  and  $b$  denote the laser wavelength, wave vector, distances from diffraction edge to mirror and laser medial axis to substrate surface, respectively. Parameter  $d$  is measured from diffraction screen to observation screen which is defined by  $d = x - x_1$ . The integral domain represents an aperture  $\Sigma$  set that contains  $y_1$  belonging negative infinity to positive infinity and  $z_1$  belonging  $b$  to infinity. The complex amplitude distribution  $\tilde{E}_1(x_1, y_1, z_1)$  of incident Gaussian beam takes the form<sup>[15]</sup>

$$\tilde{E}_1(x_1, y_1, z_1) = \frac{A_0}{w_1} \exp\left(-\frac{r_1^2}{w_1^2}\right) \exp\left[-ik\left(x_1 + \frac{r_1^2}{2R_1}\right) + i\varphi_1\right] \quad (2)$$

Where  $A_0$  is a constant factor,  $w_1$  is the laser spot radius on diffraction screen which is described by  $w_1 = w_0 \sqrt{1 + (x_1/f)^2}$ ,  $w_0$  is the waist radius of fundamental mode Gaussian beam, and  $f$  is the confocal parameter. Formulas  $R_1 = x_1 + f^2/x_1$ ,  $r_1 = \arctan(x_1/f)$ ,  $r_1^2 = y_1^2 + z_1^2$  state the radius of curvature, the phase factor, the distance from an arbitrary point at coordinate system  $z_1P_1y_1$  to origin coordinate  $O$ , respectively.

By making use of the Fourier transform of bell-type function, substituting expression 2 into equation 1, it therefore reduces to the form in the process of simplifying operations<sup>[16]</sup>.

$$\tilde{E}_1(x, y, z) = \frac{A_0 \exp(ikd)}{w_1 i\lambda d} \sqrt{\frac{\pi\lambda d R_1 w_1^2}{\lambda d R_1 - i\pi w_1^2 (R_1 - d)}} \exp\left\{\frac{i\pi\lambda R_1 - \pi^2 w_1^2}{\lambda[\lambda d R_1 - i\pi w_1^2 (R_1 - d)]} y^2\right\} \exp(-ikx_1 + i\varphi_1) \int_b^{\infty} \exp\left(-\frac{z_1^2}{w_1^2}\right) \exp\left\{\frac{i\pi}{\lambda} \left[\frac{(z - z_1)^2}{d} - \frac{z_1^2}{R_1}\right]\right\} dz_1 \quad (3)$$

As the total reflection principle illustrates, when incident wave propagates to mirror, it will create reflected wave of opposite direction but the same intensity. Similarly, the complex amplitude  $\tilde{E}_2(x, y, z)$  of reflected wave on observation screen is given by analogy. Based on scalar superposition theory, the intensity distribution in laser standing wave field is then<sup>[17]</sup>

$$I(x, y, z) = \left| \tilde{E}_1(x, y, z) + \tilde{E}_2(x, y, z) \right|^2 \quad (4)$$

Substituting equation 4, until the whole system is satisfied the steady state, the optical potential of Cr atoms in diffraction field can be written as<sup>[18]</sup>

$$U = \frac{\hbar\delta}{2} \ln \left[ 1 + \frac{I(x, y, z)}{I_s} \frac{\Gamma^2}{\Gamma^2 + 4\delta^2} \right] \quad (5)$$

Generally,  $\hbar$ ,  $\delta$ ,  $\Gamma$  and  $I_s$  are the planck constant, laser field detuning, natural linewidth and saturated absorption intensity of the atom, respectively.

## RESULTS AND ANALYSIS

As the model of Fresnel straight edge diffraction shows, two special parameters  $x_1$  and  $b$ , both of them could affect the forming process of laser field. In order to research these disturbance factors, we prepare to simulate the 3-D constructions of optical potential, which provide more intuitive, abundant and comprehensive parameters to set up the diffraction standing wave field. In experimenting we apply the chromium atom  ${}^7S_3 \rightarrow {}^7P_4^o$  transition to computational analysis, while the corresponding resonant laser wavelength equals 425.55 nm, also,  $\delta = 200 \times 2\pi\text{MHz}$ ,  $I_s = 5 \times 2\pi\text{MHz}$ ,  $I_s = 85\text{W}/\text{m}^2$ ,  $\omega_0 = 0.1\text{mm}$ .

### The influence of the distance from diffraction edge to mirror

This paper will investigate the change in parameter  $x_1$  before substrate position needs to satisfy two conditions. First, mirror M stays the waist radius of Gaussian beam, and then the vertical direction. Second, make sure that the longitudinal position of substrate surface overlaps with laser medial axis. Among characteristic parameters of optical potential,  $U_{\max}$ ,  $U_{\min}$  and  $Z$  represent the peak, valley, ordinate corresponding with valley value. Especially as an evaluation criterion,  $C$  is the result of dividing peak value by valley value in straight edge diffraction field (TABLE 1).

As the parameter  $x_1$  increases, it can be found that there are four aspects of the characteristic trends. Firstly, peak values gradually decrease so that the ability to capture the chromium atoms is weakened simultaneously. Secondly, in contrast to the changes in peak values, valley values trend towards enlarger accompanied with minor

fluctuations, which lead to the thickened bottom of deposition gratings. Thirdly, peak-to-valley ratio  $C$  will achieve a maximum limit when the disturbance factor  $x_1$  equals 0.51 cm, that is, the best standing wave construction. With removing substrate edge away from mirror, not only peak-to-valley ratio but also the quality of standing wave becomes worse gradually, meanwhile, it explains the reason for which substrate should maintain a minimum distance by keeping close to the laser beam waist center. Fourthly, every  $Z$  value is greater than 0 and the extent of its deviation rises, hence, the dipole force induces Cr atoms to gather in valley above substrate surface which is decided by the distance from diffraction edge to mirror. Finally, the diffraction field converges Cr atoms in advance, thus atomic trajectories deviate from the original directions and deposition patterns are deteriorated accordingly.

TABLE 1 : The comparison of major parameters in optical potential.

$x_1 / \text{cm}$	$U_{\max} / \mu\text{eV}$	$U_{\min} / \mu\text{eV}$	$C$	$Z / \text{m}$
0.21	0.4289	5.4773e-04	783	2.5533e-05
0.51	0.3934	1.2948e-05	30385	3.6597e-05
1.02	0.3434	2.4048e-04	1428	4.7662e-05
2.00	0.2769	9.2521e-04	299	5.9577e-05
4.26	0.2046	6.1850e-03	33	6.9790e-05

While the substrate is moved along  $x$  direction, the optical potential structure is shown (Figure 2). By comparing the four pictures, it can be seen that the impact of diffraction effect will decrease with increasing distance from diffraction edge to mirror. Transverse optical potential takes on the shape of standing wave, the period of which is half of laser wavelength, and the structure is all far away from diffraction edge as a result of the growth of parameter  $x_1$ . Longitudinal optical potential structure seems like Gaussian distribution and its light propagation area, the region of which  $z$  is greater than 0, shows an oscillating phenomenon which appears to recede with the increase of parameter  $x_1$ .

### The influence of the distance from laser medial axis to substrate surface

From the Figure 3, it shows that the influence degree of optical potential by substrate's longitudinal position through a comparison to an ideal standing wave field. This paper applies numerical analysis method to parameter  $b$  belonging  $-3\omega_0$  to  $3\omega_0$ , and then find that when parameter  $b$  is less than  $-2\omega_0$ , laser standing wave has no interference whether diffraction effect is considered or not. Moreover, due to the fact that substrate blocks most of Gaussian beams, so the maximum depth of optical potential is too small to capture Cr atoms when parameter  $b$  is greater than  $2\omega_0$ . Furthermore, diffraction effect

plays a large role centrally in the remaining region ranging from  $-2\omega_0$  to  $2\omega_0$ <sup>[19]</sup>.

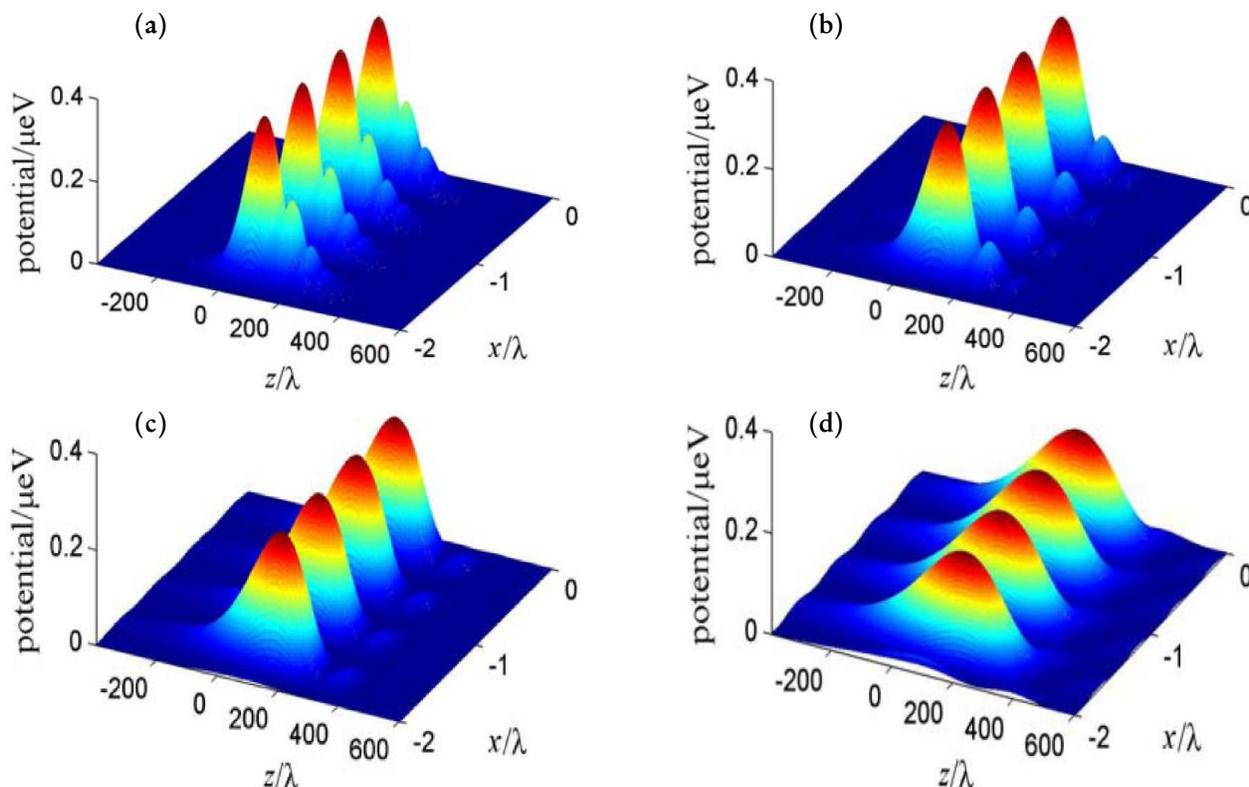


Figure 2 : 3-D distribution of optical potential in straight edge diffraction field under different parameters  $x_1$ . Figures 2(a), (b), (c) and (d) show optical potential structure when the sole variable values equal 0.51 cm, 1.02 cm, 2.00 cm, 4.26 cm, respectively.

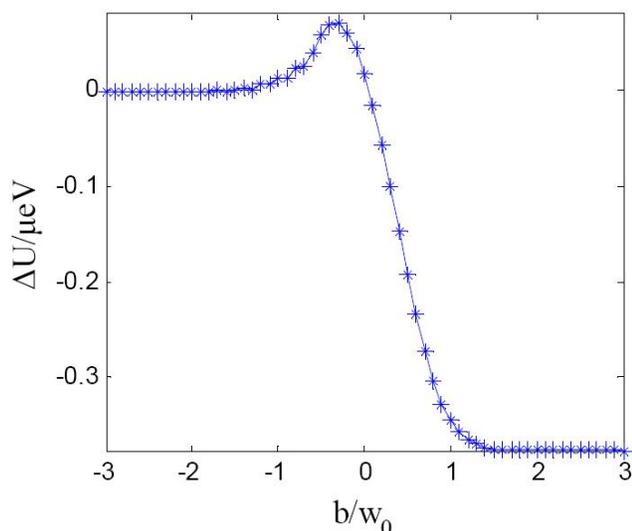


Figure 3 : The influence of parameter  $b$  on optical potential  $\Delta U$ . Vertical coordinate stands for the peak difference between diffraction field and ideal field.

The relationship between parameter  $b$  and  $Z$  is shown (Figure 4). When parameter  $b$  is selected in the range from  $-0.65\omega_0$  to  $2\omega_0$ , parameter  $Z$  has a variation of direct proportion with  $b$ , but their distances go down from 0.04 mm to 0.02 mm. It indicates that, the ultimate location of Cr atoms focusing will get closer to substrate surface, whereas an objective rule that parameter  $Z$  is greater than  $b$  always exists throughout the rising process

of substrate. As a result, parameter  $b$  is another contributive factor which Cr atoms are eventually deposited above the substrate.

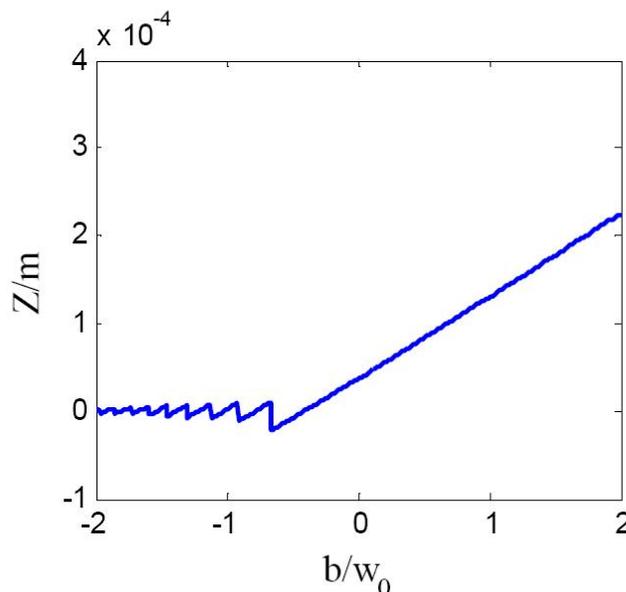


Figure 4 : The ordinate  $Z$  corresponding with valley value as a function of the distance  $b$ . It reflects an extent of deviation from the ultimate location of Cr atoms focusing to substrate surface.

While the substrate is moved along  $z$  direction, 3-D simulation of optical potential is shown (Figure 5). Through

the above analysis, the distance from laser medial axis to substrate surface is limited between  $-2w_0$  and  $2w_0$  for research. When substrate is moved upwards, transverse potential structure shifts to the orientation of diffraction edge, and longitudinal structure generates irregular fluctuations owing to the impact of diffraction effect. As described in

Figure 5(b), at this time, the oscillation amplitude has leveled off in the shaded area ( $z$  is less than  $b$ ), while intensified in the light propagation area ( $z$  is greater than  $b$ ) and then slowly weakened with the ascending movement of the substrate, finally, diffraction result has appeared more and more blurring.

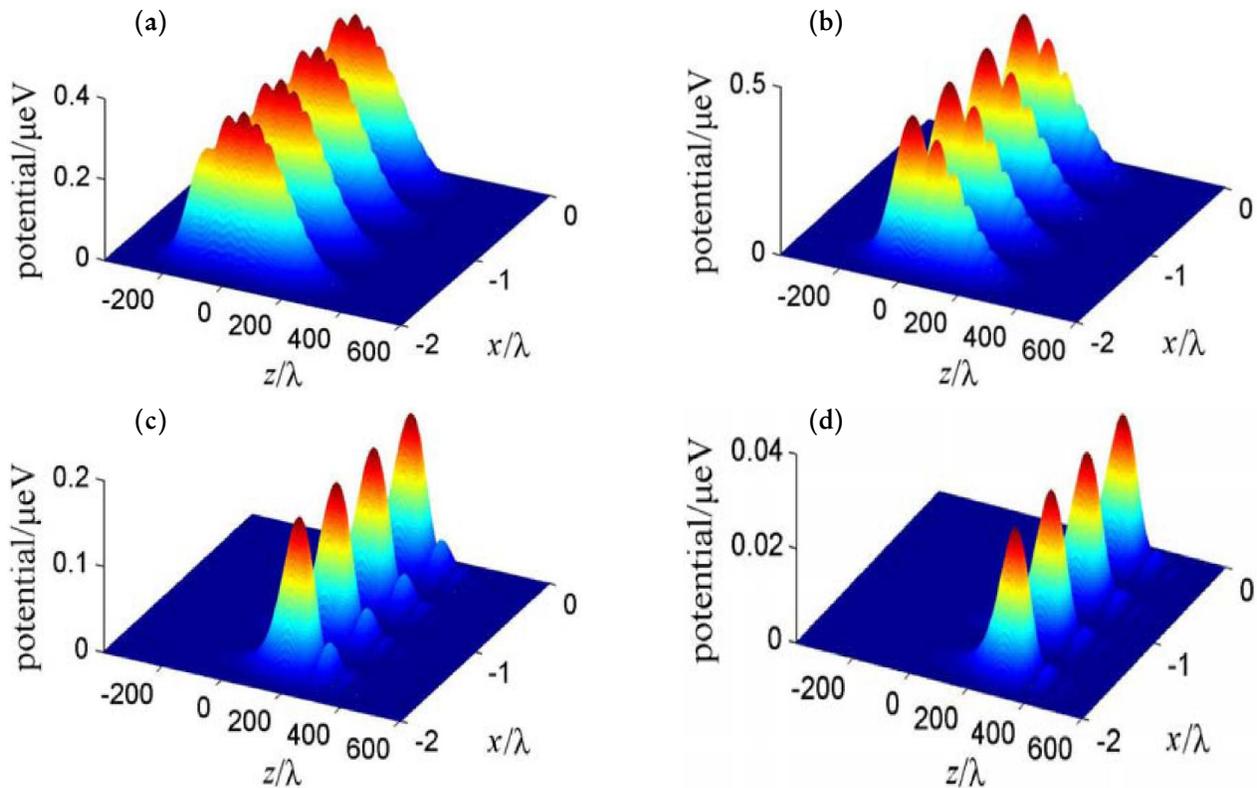


Figure 5 : 3-D distribution of optical potential in straight edge diffraction field under different parameters  $b$ . Figures 5(a), (b), (c) and (d) show optical potential structure when the sole variable values equal  $-w_0$ ,  $-0.5w_0$ ,  $0.5w_0$ ,  $w_0$ , respectively.

### CONCLUSION

In this paper, taking into account the substrate edge, the model of Fresnel straight edge diffraction is built in the fundamental mode Gaussian laser standing wave. Another model is proposed in Ref.<sup>[20]</sup>. Through 3-D simulation analysis, it can be found that, for the sake of the minimum distance between diffraction edge and mirror, substrate should be placed adjacent to mirror as close as possible, so that the maximum potential depth is attained, and Cr atoms are deposited at the nearest location above the substrate surface, meanwhile, it decreases the influence of diffraction effect in the deposition experiment. What's more, adjusting to transverse and longitudinal positions of the deposition substrate, the final deposition place is no longer on the substrate surface but above it. However the analysis in this paper only qualitative, the actual trajectories and deposition gratings about Cr atoms in 3-D space will be studied in the near future based on straight edge diffraction effect. And the structures of nano-patterns are described in the Refs.<sup>[21-24]</sup>.

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