

Blazed Nanostructure Gratings for Electron and Atom Diffraction

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Van der Waals potentials and image charge potentials are shown to have a similar effect on the diffraction of atoms and electrons from free-standing nanostructure gratings. Asymmetric (i.e. blazed) diffraction patterns are demonstrated for both atoms and electrons, and are attributed to atom-surface and electron-surface interaction potentials.

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Nanofabricated transmission gratings for electron diffraction are now available [1, 2] and may serve as coherent beam splitters for electron interferometry just as they already do for atom interferometry. For electron beams with kinetic energy less than 10 keV, nanostructures offer several advantages over solid crystal gratings, for example larger transmission, less inelastic scattering, and the possibility of engineering blazed diffraction gratings. Blazed gratings enhance the intensity of a particular diffraction order, and can be used to make more efficient beam splitters for interferometry. To design a blazed nanostructure grating, we must first understand and then control the phase shifts for matter waves that are caused by interactions with the nanostructure. To learn how different interactions (e.g. image charge or van der Waals potentials) affect the design, here we compare electron and atom diffraction from similar nanostructures. With simulations we show how phase shifts can lead to asymmetric diffraction patterns, and we present electron and atom diffraction data that supports this theory.

The main goal of this work is to study how diffraction from nanostructure gratings can be modified by conservative potentials that cause coherent phase shifts. If the interactions between matter waves and the gratings are too strong, then the incident flux is spread out over many diffraction orders. On the other hand, if the interactions can be controlled, then we can produce an optimal blazed grating. The maximum possible asymmetry between the +1 and -1 orders, and the maximum efficiency for diffraction into the +1 order are quantified both for atoms and electrons. In the future, similar work can be extended to measure material properties such as the electric permittivity of the grating bars, and also to study decoherence induced by the nanostructure surfaces.

Silicon nitride transmission gratings with a 100 nm period have been used for x-ray diffraction [3], atom diffraction [4], molecule diffraction, and atom interferometry [5]. More recently the 40-nm wide free-standing grating bars

have been coated with ~ 1 nm of gold metal and then used to diffract electrons [1, 2]. In general, the grating bars absorb electrons, atoms, and x-rays, and the channels between bars transmit these kinds of waves. For the matter waves, due to the electron-surface (image charge) or atom-surface (van der Waals) potentials, passage through the gratings channels causes a phase shift that depends on position. Hence, the gratings can be described by a complex transmission function, and this offers the possibility of asymmetric (i.e. blazed) diffraction demonstrated here. Asymmetric diffraction patterns have been detected and analyzed for atom diffraction [6], and a similar analysis is presented here for electron diffraction.

The de Broglie wave optics is indeed similar for electrons and atoms even though the electron-surface and atom-surface potentials depend on quite different mechanisms and depend differently on distance to a surface. Surprisingly, the phase shifts for electrons and atoms due to passage through the center of the channels (i.e. 30 nm from each wall) are similar in magnitude even though the electron-surface and atom-surface interaction potentials are different by five orders of magnitude. This accidental similarity occurs because the velocity for 0.1 eV atoms and 500 eV electrons discussed here nearly compensates for the difference in potential. Another similarity is that the phase front curvature has the same sign for electrons and atoms, because both are attracted to surfaces.

The atom-surface van der Waals interaction can be approximated by the sum of interactions with each wall,

$$V_a(x) = -\frac{C_3}{r_1^3} - \frac{C_3}{r_2^3} \quad (1)$$

where x is the transverse coordinate inside the channel, $r_{1(2)}$ is the magnitude of the distance to each wall, and C_3 is the van der Waals coefficient. For sodium atoms and a silicon nitride surface, C_3 has been measured to be approximately 2.7 meVnm^3 [4]. For electrons, the

electron-surface interaction potential is approximately

$$V_e(x) = -\frac{C_1}{r_1} - \frac{C_1}{r_2} \quad (2)$$

where C_1 is due to an image charge associated with each wall, and has been measured to be approximately 3 Vnm for gold-coated silicon nitride grating bars [1]. For 60 nm wide channels between parallel walls, the potential energy for atoms and electrons as a function of position is shown in Figure 1a. In the center of the channel the two potentials are different by a factor of nearly 10^5 .

Phase shifts due to these potentials are calculated in the WKB approximation to first order in potential over total energy, (V/E), by

$$\phi(x) = -\frac{V(x)\ell}{\hbar v} \quad (3)$$

where ℓ is the depth of the grating, \hbar is Planck's constant divided by 2π and v is the velocity of the particles. Phase

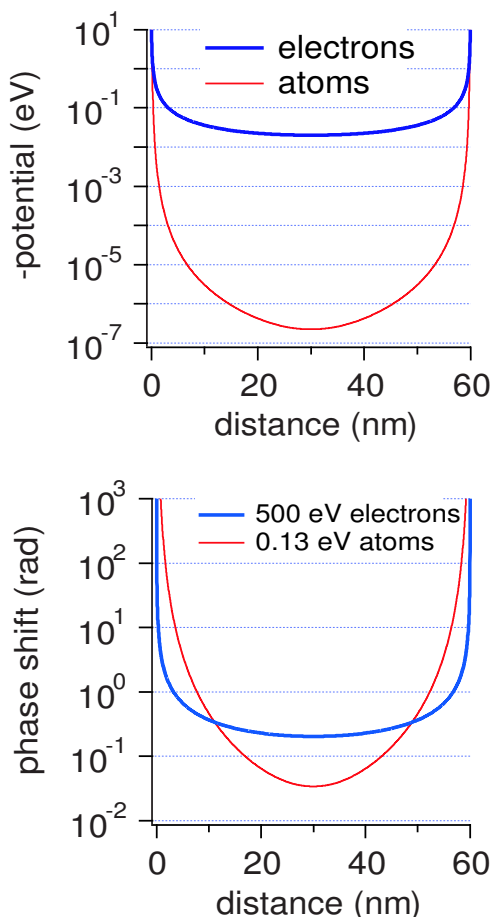


FIG. 1: (Top) Potential energy for electrons and atoms as a function of position in a 60nm wide channel between parallel sided grating bars. (Bottom) Phase shift for electron waves and atom waves after propagating 100nm in the channel.

shifts for atom and electron waves are shown in Figure 1b. The role of $\phi(x)$ in atom diffraction has been studied in several papers [4, 6–9] but the comparison to electrons is new. It is noteworthy that in the center of the channel, the phase shift is within an order of magnitude for electrons and atoms.

It was shown in [4] that the diffraction envelope is given by a Fourier transform of the single slit diffraction. In this case the slit is a channel, and the phase $\phi(x)$ makes the transmission function complex. Using this fact, the diffraction envelopes for electron and atom waves are plotted in Fig. 2 for the case of normal incidence on a grating with parallel-sided channels. It was also shown in [4] that the intensity of the j^{th} diffraction order is most strongly affected by regions in the channel where the the spatial derivative of phase matches the condition for constructive interference in the j^{th} order, namely:

$$\frac{d\phi(x)}{dx} = jk_g, \quad (4)$$

where k_g is grating wavenumber. Hence, the diffraction pattern envelopes shown in Fig. 2 should look similar to the extent that the spatial derivative of the phase profiles shown in Fig. 1b for electrons is similar to that for atoms.

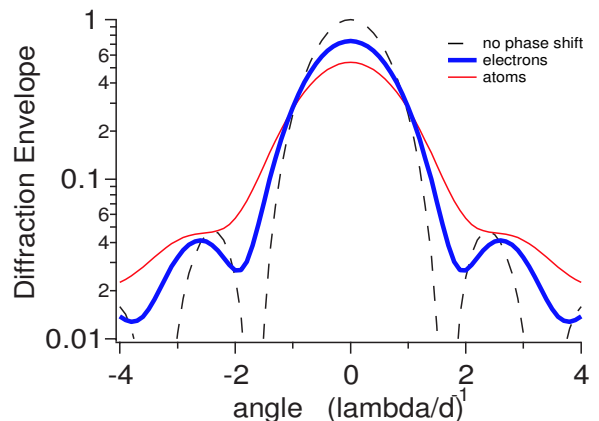


FIG. 2: Far field diffraction patterns for atoms (thin red) and electrons (thick blue) and for reference, particles that do not interact with the grating bars (dotted black)

Asymmetric (i.e. blazed) diffraction patterns result from skewed phase profiles. In principle, there are several ways to make blazed transmission gratings by designing grating bar structures that create an asymmetric potential energy as a function of position in the channels. For example, different lengths ℓ , different material coatings, or different shapes for opposite channel walls can each cause an asymmetry. To begin, we explore how trapezoidal grating bars used at non-normal incidence make a blazed gratings since we already have nanostructures with the cross section geometry shown in in Fig-

ure 3 (top). When used at normal incidence, these bars make symmetric phase profiles, but when used at non-normal incidence, the result is asymmetric phase profiles, as shown in Figure 3 (middle). The asymmetric far-field diffraction that results from this single slit transmission phase is shown in Figure 3 (bottom). For a grating rotated with the opposite angle of incidence, the asymmetry reverses. Furthermore, to test this theory, we predict that gratings rotated 180 degrees, so they have the same angle of incidence, but oppositely oriented trapezoidal bars as shown in Figure 4 (top) also reverses the asymmetry. Data shown in figures 5 and 6 confirm this prediction.

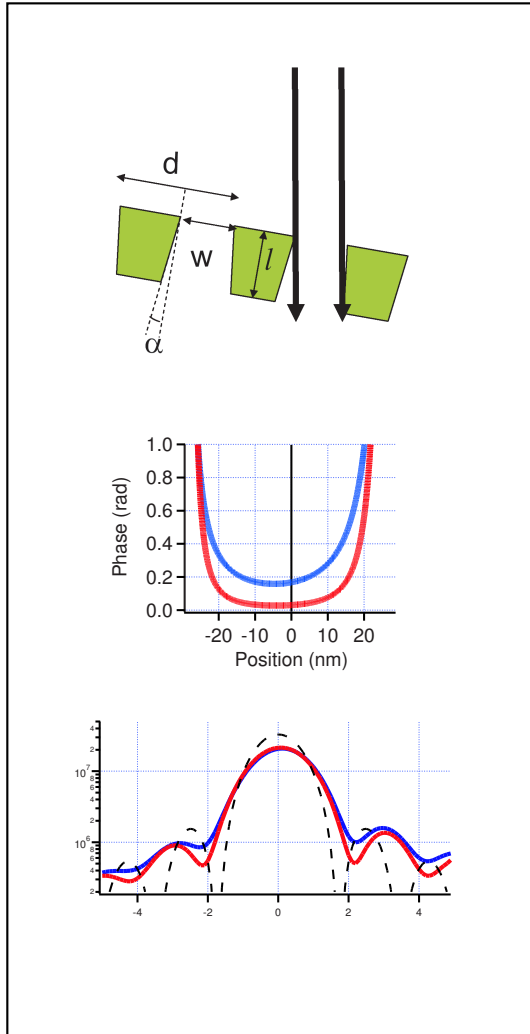


FIG. 3: Trapezoidal grating bars oriented so incident beams have an angle of incidence of 5 degrees (top). The phase profiles that result from passage through trapezoidal channels at this angle are shown for atoms in red and electrons in blue (middle). The far-field diffraction envelopes that result from these phase profiles is shown for atoms in red and electrons in blue (bottom).

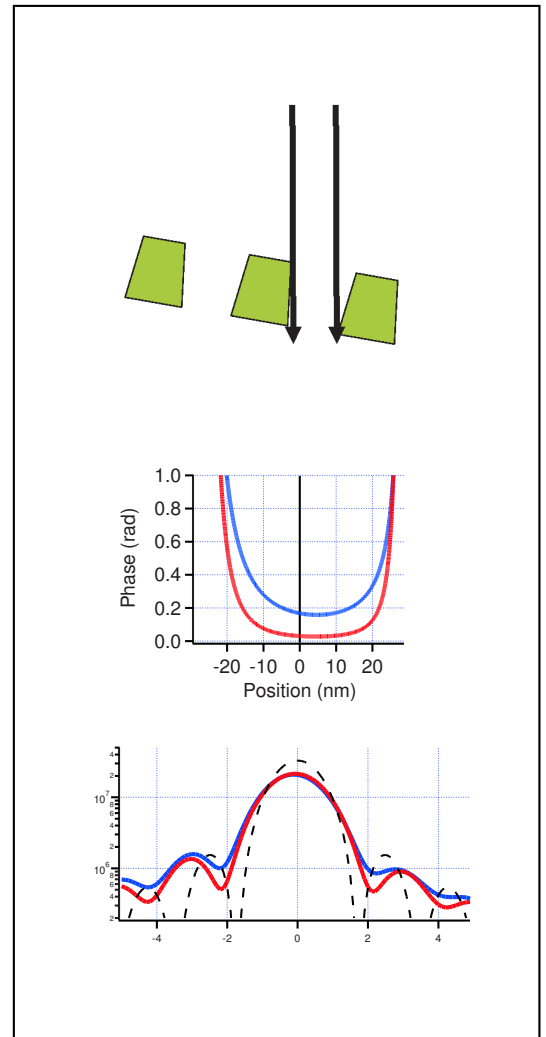


FIG. 4: Trapezoidal grating bars oriented so incident beams have an angle of incidence of 185 degrees (top). The phase profiles that result from passage through trapezoidal channels at this angle are shown for atoms in red and electrons in blue (middle). The far-field diffraction envelopes that result from these phase profiles is shown for atoms in red and electrons in blue (bottom).

Electron diffraction patterns obtained with electron beams incident at non-normal angles on a grating are shown in Figure 5. Atom diffraction from a similar grating is shown in Figure 6. Both electrons and atoms can produce asymmetric diffraction patterns, as predicted, if the grating is not used at normal incidence.

Furthermore, rotating the grating by 180 degrees reverses this asymmetry. This supports the theory that the asymmetric diffraction pattern is due to the nanoscale geometry of the grating bar (in this case the trapezoidal wedge angle) in addition to the angle of incidence.

The diffraction asymmetry can be larger for electrons than atoms because of the different power law for the

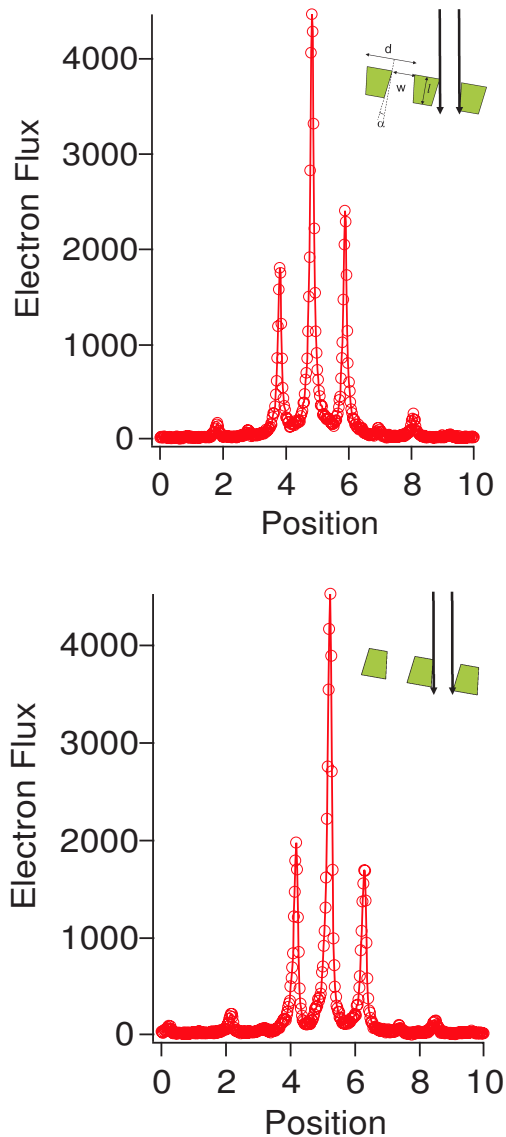


FIG. 5: Electron diffraction data with an angle of incidence of 5 degrees (top) and 185 degrees (bottom). Lines are shown between data points.

potentials. Using the idea that the region in the channel where $\phi'(x) = jk_g$ contributes constructively to the j th order, we may examine the range in the channel, Δx_{max} , for which $\frac{1}{2} < j < \frac{3}{2}$ to estimate how much stronger the +1 order can be. This only gives a heuristic way to determine how much the potential can influence the asymmetry, but it gives the correct trend for different potentials. Consider a power law for the potential so that $V = -C_p/r^p$ then the gradient in phase is $\phi' = \phi'_p/r^{p+1}$ where the coefficient ϕ'_p can be determined using Eq 3. Furthermore, if we create a maximally asymmetric channel with a wall on one side of length ℓ and a wall

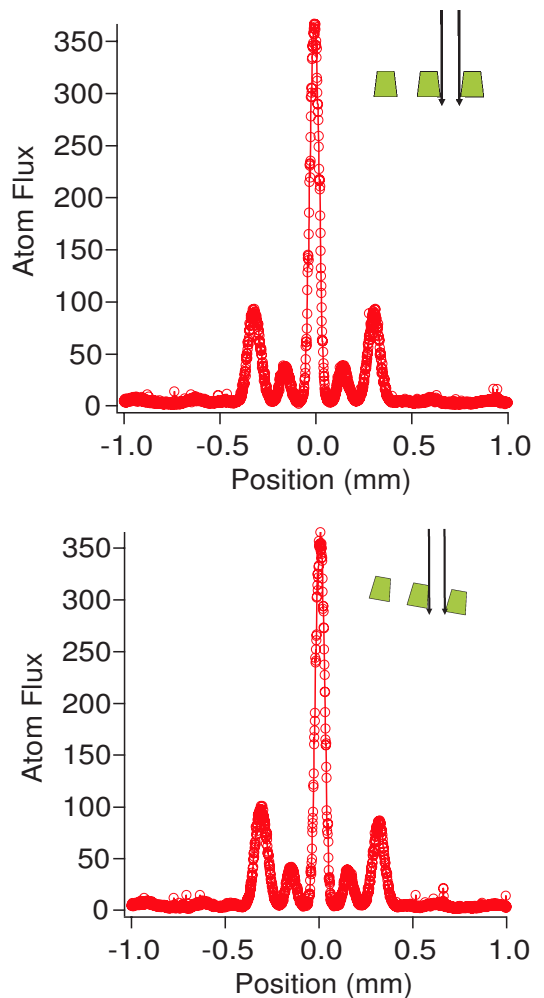


FIG. 6: Atom diffraction data with an angle of incidence of 180 degrees (top) and 185 degrees (bottom). Lines are shown between data points.

on the other side with zero length, i.e. triangular grating bars with one wall parallel to the incident beam, then we can adjust the potential coefficient C_p such that the gradient in phase at the far side of the channel from the wall can be set to $\phi' = \frac{1}{2}k_g = \phi_p/w^{p+1}$. This determines $\phi'_p = k_g w^{p+1}/2$, and gives the maximum range Δx_{max} for which the $\phi' = (1 \pm \frac{1}{2})k_g$. This is $\Delta x_{max} = w[1 - 3^{-1/(p+1)}]$. For atoms $p = 3$ and $\Delta x_{max} = 0.24 w$; for electrons $p=1$ and $\Delta x_{max} = 0.42w$. This supports the claim that electron diffraction can be more asymmetric than atom diffraction.

Numerical simulations show that the maximum asymmetry defined as

$$asym = \frac{(I_{+1} - I_{-1})}{(I_{+1} + I_{-1})} \quad (5)$$

for electrons can be $asym = xxx$ and for atoms is $asym = xxx$.

One might ask, can we distinguish between different power law potentials just by observing the diffraction pattern. To get a graphical answer to this question, we have plotted the diffraction envelope for five different power law potentials with the coefficients C_p chosen so that the 0 and ± 1 order diffraction peaks have equal intensity. Then, we see that that higher orders do not match.

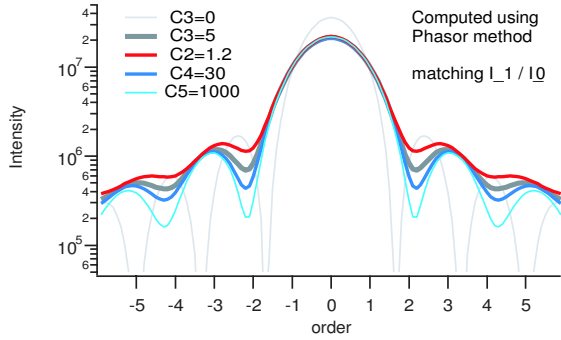


FIG. 7: Diffraction envelopes for matter waves that have potentials given by $V = C_p/r^p$ shown for values of $p=0,1,2,3,4,5$. The coefficients C_p have been chosen to match the ratio of zeroth order to first order intensity

Blazed grating proposals.

In conclusion, we have explained the experimental asymmetry in the diffraction pattern for both electrons and atoms. We have

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- [1] G. Gronniger, B. Barwick, T. Savas, A. Cronin, D. Pritchard, and H. Batelaan, submitted to PRL (2005).
 - [2] A. Cronin, B. McMorran, and T. Savas, submitted to Ultramicroscopy (2005).
 - [3] (????).
 - [4] J. Perreault, A. Cronin, and T. Savas, arXiv:physics/0312123 (2003).
 - [5] T. D. Roberts, A. D. Cronin, D. A. Kokorowski, and D. E. Pritchard, Physical Review Letters **89** (2002).
 - [6] A. Cronin and J. Perreault, Phys. Rev. A **70**, 043607 (2004).
 - [7] R. E. Grisenti, W. Schollkopf, J. P. Toennies, G. C. Hegerfeldt, and T. Kohler, Phys. Rev. Lett. **83**, 1755 (1999).
 - [8] R. E. Grisenti, W. Schollkopf, J. P. Toennies, J. R. Manson, T. A. Savas, and H. I. Smith, Phys. Rev. A **61**, 033608 (2000).
 - [9] R. Bruhl, P. Fouquet, R. E. Grisenti, J. P. Toennies, G. C. Hegerfeldt, T. Kohler, M. Stoll, and D. Walter, Europhys. Lett. **59**, 357 (2002).