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Multiphysics Modeling of Grating Chips for Magneto-Optical Trapping of Atoms

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Abstract: We present a modeling method that incorporates full-wave electromagnetic simulations and radiation force calculations to evaluate the performance of grating chips for compact megneto-optical traps (MOTs). © 2022 The Author(s)

Grating chips have been demonstrated to be a viable platform for trapping cold atoms, and have a significantly reduced experimental footprint compared to a standard three-dimensional magneto-optical trap (MOT) [1]. However, evaluating grating chips can be challenging, as illustrated in [2]. Here, we propose a multiphysics approach which builds on previously proposed figures of merit, such as beam overlap volume, balancing efficiency [2] [3] and polarization of the diffracted beams [4] that allows us to correlate (fabrication and degradation) errors of the grating chip with MOT performance.

As an example, we evaluated a two-dimensional grating chip we recently fabricated to simultaneously trap ^{87}Rb and ^{133}Cs atoms, corresponding to incident beam wavelengths, $\lambda_{inc} \sim 780$ nm and $\lambda_{inc} \sim 852$ nm, respectively. Fig. 1 illustrates the grating chip design.

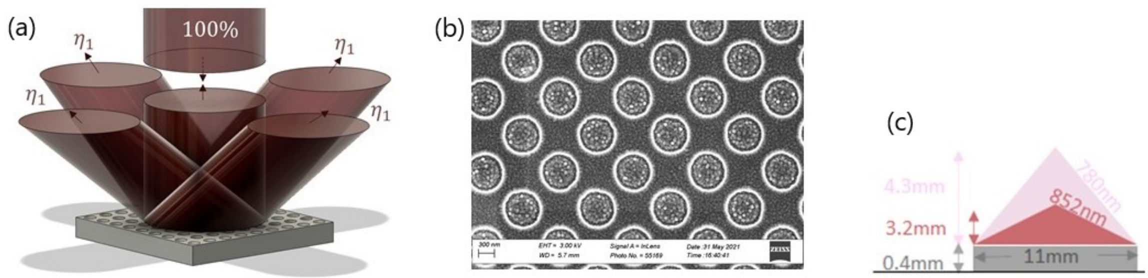

Fig. 1. (a) For an isotropic incident beam, the grating chip that we evaluated produces first-order diffracted beams at azimuthal angles $\phi = 0,\ \pi/2,\ \pi,\ 3\pi/2$ and grating angle $\theta = 53^o$ (at $\lambda_{inc} \sim 780$ nm; the other wavelength not shown). The intensity efficiency of first-order diffracted beams is $\eta_1 \sim 23\%$ and for zero-order diffracted beam is $\eta_0 \sim 0.7\%$. (b) SEM image of the fabricated grating structure. (c) Illustrates the beam overlap regions for both λ_{inc}.

We initially obtain the intensity and polarization of diffracted beams of the grating using finite-difference time-domain (FDTD) simulations. Using the output of the FDTD, we numerically determine the trapping-force profile on an idealized ^{87}Rb atom, and optimize the grating chip design. Post-fabrication, measured the intensity and polarization properties of the diffracted beams and used these measurements to numerically calculate the trapping-force profile. We are able to compare the force calculations based on experimental data and based on FDTD simulations, and thus determine the expected impact of fabrication errors on the properties of the MOT.

The FDTD simulation provides the polarization states of the diffracted beams in terms of complex electric-field amplitudes in the linear basis ($\mathbf{\tilde{E}_s}$ & $\mathbf{\tilde{E}_p}$), which we then transform into the spherical basis to enable radiation force calculations. We first transform the linear basis into elliptical basis by determining the auxiliary angle α, given by $\tan\alpha = |\mathbf{\tilde{E}_s}|/|\mathbf{\tilde{E}_p}|$. Subsequently we determine the ellipticity angle $\chi = \sin^{-1}[(\sin 2\alpha)\sin\delta]/2$, where δ denotes the phase angle between $\mathbf{\tilde{E}_s}$ and $\mathbf{\tilde{E}_p}$ [5]. In the spherical basis, we define three unit vectors corresponding to each light beam: $\varepsilon_{\mathbf{0}} = (\theta,\phi)$; $\varepsilon_{\mathbf{a}} = (\theta+\pi/2,\phi)$ and $\varepsilon_{\mathbf{b}} = \varepsilon_{\mathbf{0}} \times \varepsilon_{\mathbf{a}}$. Overall, each light beam's polarization vector in the spherical basis is denoted by $\varepsilon = (\cos\chi)\varepsilon_{\mathbf{a}} + i(\sin\chi)\varepsilon_{\mathbf{b}}$.

To demonstrate the technique, we examine the MOT obtained for the D2 transition line of ^{87}Rb atoms using the grating chip illustrated in Fig. 1. The net radiation force on an idealized, two-level atom for the transition

$J_g = 0 \rightarrow J_e = 1$ is given as:

$$\mathbf{F} = \frac{\hbar k \Gamma}{2} \sum_{j=1}^{N} \sum_{q=-1,0,1} \frac{\frac{I_{jq}}{I_s}}{1 + \frac{4(\Delta - \delta_q)^2}{\Gamma^2} + \frac{I_T}{I_s}} \hat{k}_j \tag{1}$$

where $k = 2\pi/\lambda_{inc}$ is the wave-number; $\Gamma = 2\pi \times 6.07$ MHz is the natural linewidth and $I_s = 3.58$ mW/cm^2 is the average saturation intensity [6]; $\delta_q = \frac{q\mu_B g_e B}{\hbar}$ where μ_B is Bohr magneton, g_e is the excited state Landé factor and B is the magnetic field intensity; j identifies each of the $N = 6$ beams illustrated in Fig. 1 (a). $I_{jq} = I_j |\varepsilon_j^* . \varepsilon_{\mathbf{B}q}|^2$, where ε_j is the beam's polarization vector as determined above and $\varepsilon_{\mathbf{B}q}$ is the magnetic field polarization vector expressed in the spherical basis; $I_T = \sum_j \sum_q I_{jq}$. We set up our simulations with commonly-used parameters for achieving a ^{87}Rb MOT: a σ polarized plane wave with $\lambda_{inc} \sim 780$ nm, detuning $\Delta = -2\Gamma$, intensity $I_{inc} = 3I_s$ incident normally along with $dB/dz = 10$ G/cm.

Using the intensity and polarization states of the diffracted beams obtained from the FDTD simulation, we determine the trapping-force profiles (blue curves in Fig. 2). For post-fabrication evaluation of the grating chip, we measured the intensity of the diffracted beams and determined their χ by passing each beam through a polarizer to record the minimum and maximum power while rotating the polarizer, thereby calculating $\chi = \tan^{-1}[-\sqrt{P_{min}/P_{max}}]$ and hence determined ε for each beam. Using these experimental values, we obtained a corresponding set of trapping-force profiles, illustrated by red curves in Fig. 2.

We also compared the expected volume of the MOTs obtained via both the trapping-force profiles. The spatial extent of a MOT can be estimated as a Gaussian distribution, so the potential energy near the trap centre can be denoted as $U(r) \sim -\frac{1}{2} f_r r^2$, where f_r is the linear slope of the force vs r curve and $r = x, y$ or z. The atom density distribution scales as $n(r) = n_o e^{\sum_r -U(r)/K_B T}$, where K_B is the Boltzmann constant and T denotes the atom temperature. The $1/e^2$ width of the atom distribution is $\sigma_r = 4\sqrt{K_B T / f_r}$ and the volume is $\prod_{r=x,y,z} \sigma_r$. For an arbitrarily chosen $T = 730\,\mu$K, the force profiles generated using the FDTD simulation suggest a MOT volume ~ 2.4 mm^3 with $\sigma_z \sim 0.8$ mm, while the experimentally determined data suggests a MOT volume ~ 2.9 mm^3 with $\sigma_z \sim 0.8$ mm. The trapping-force profiles, along with the MOT volumes, are in close agreement, while σ_z is within the beam overlap volume illustrated in Fig. 1(c).

In conclusion, we demonstrated a multiphysics method for evaluating a grating chip for atom-trapping experiments, while providing a direct figure of merit for evaluation.

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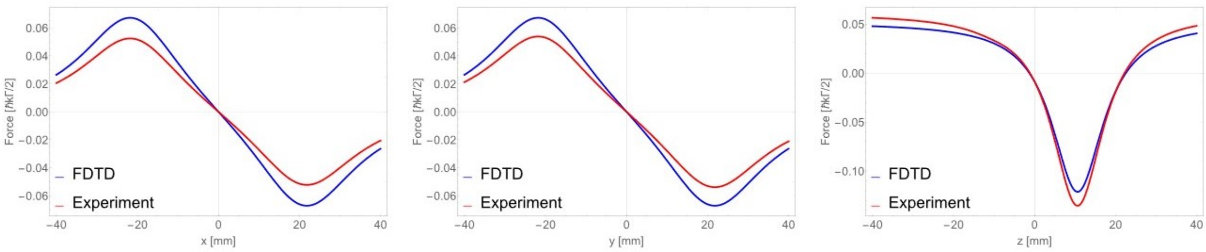

Fig. 2. Trapping force vs. distance from the MOT center for D2 transition of ^{87}Rb atom obtained using Eqn. 1. The blue curves are the trapping-force profiles obtained using FDTD simulations for the fields while the red curves are the trapping-force profiles obtained by simulating forces based on optical measurements of fabricated gratings.

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