Feasibility of Single Atom Imaging in an Optical Lattice

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Contents

1. Introduction.................................................................................................................................. 1

2. Confocal and whole-field-of-view imaging .................................................................................... 3
   2.1. 405 nm and 767 nm transitions .......................................................................................... 5
   2.2. Heating rate in the lattice ................................................................................................. 10
       2.2.1. Optical density ......................................................................................................... 11
   2.3. Optical resolution .............................................................................................................. 11
       2.3.1. Pixellation effect ...................................................................................................... 14
   2.4. Experimental reports ......................................................................................................... 15
   2.5. Optical Lattice .................................................................................................................. 16
       2.5.1. Néel temperature ..................................................................................................... 18
   2.6. S/N and required photon number ..................................................................................... 21

3. Imaging window .......................................................................................................................... 26
   3.1. Sapphire and fused quartz ............................................................................................... 27
   3.2. Strehl ratio and Marechal criterion .................................................................................... 28
   3.3. Rupture .............................................................................................................................. 29
   3.4. Bending .............................................................................................................................. 30
   3.5. Birefringence in sapphire ................................................................................................. 32
   3.6. Effect of index of refraction ............................................................................................. 34
   3.7. Summary ............................................................................................................................ 38

4. Microscope objectives ............................................................................................................... 39
4.1. CTF and MTF function ..................................................................................... 42
4.2. Change of contrast by nonstandard coverslips ................................................. 43
4.3. Summary ........................................................................................................... 45

5. Conclusions ......................................................................................................... 47

References: .............................................................................................................. 48
1. Introduction

The Hubbard model for fermions describes many-body physics of electrons in solids and provides an essential description of the quantum physics of superconductivity. It was shown by Jaksch et al. that optical lattice of cold atoms is a realization of Hubbard model [1]. In cold atom experiments, controllability of parameters like lattice intensity and detuning from Feshbach resonance is a powerful tool to further shed light on high temperature superconductivity, Mott-insulating phases and interacting spin systems [2,3,4].

Fermionic atoms with attractive interaction will undergo a phase transition to give S-wave superfluidity. Superfluidity in cold atoms is the counterpart of superconductivity in solids. Lattice potential enhances the interaction strength and increases the transition temperature by some orders of magnitude compared to weakly confined atoms [2].

Due to the phenomenon of Feshbach resonance, by applying a magnetic field, we are able to couple different collisional channels of atom to efficiently control the interaction of spin species; even change it from attractive to repulsive.

In the case of weakly repulsive interactions, depending on the filling fraction of the lattice at low temperature, antiferromagnetic or d-wave superfluid phases appear. D-wave pairing is stated as the possible mechanism for high temperature superconductivity in cuprates [2].

Experimental quantum simulation of different many-body systems is possible with this high controllability of interactions in cold atoms in optical lattices. So far, phase coherence and hence, superfluidity have been explored by the observed interference peaks and vortex lattices after the ballistic expansion of cold cloud from optical lattices [5]. In order to investigate the antiferromagnetic phase of a weakly repulsive Fermi degenerate gas in an optical lattice, we need to achieve single atom imaging in a unity filled lattice. The critical temperature of paramagnetic to ferromagnetic phase transition (Néel temperature) is of the order of one nano-Kelvin and is inversely proportional to the
square of the lattice spacing. Because of this extremely low temperature, we are interested in obtaining the minimum possible lattice spacing. In this thesis, we explore the possibility of this high resolution imaging and determine restrictions on it.

In chapter 2, we discuss in general, the possibility of confocal and whole-field-of-view imaging and compare their requirements. In sections 2.1 and 2.2, master equations for $^{40}$K atom are solved and heating rates for different transitions are derived. In section 2.3, optical resolution of an objective system is defined and the effect of pixellation on resolution is explored. In 2.4, an experimental report of the resolution of an optical system for imaging two single atoms is presented. In 2.5, we discuss critical temperature of antiferromagnetic transition (Néel temperature). We derive the restriction it imposes on the detuning of a near detuned optical lattice and the maximum possible number of scattering events for each atom before leaving the lattice. As a summary, in 2.6, the possibility of different kinds of imaging for required degree of correct detection is shown. For each kind of imaging, the required number of scattered photons by each atom is derived and compared with the maximum allowed number.

In chapter 3, we will address the problem of optical aberration due to the imaging window. Different sources of aberration are discussed and the requirements for the imaging window are given.

Finally in chapter 4, we will briefly explain different choices of objective lens and the possibility of using microscope objectives for our imaging system.
2. Confocal and whole-field-of-view imaging

Imaging techniques for cold atom clouds are categorized by detection or stage of imaging. Usually, we shine a laser light on atomic cloud and detect partially absorbed light (absorption imaging) or fluorescence photons (fluorescence imaging). Imaging can be done in-situ or after ballistic expansion (time of flight imaging). In this thesis, we are interested in in-situ imaging of single atoms in the lattice. Another factor that can be engineered in imaging is the illumination geometry. Mostly, people utilize laser light with diameter greater than the cloud size. Confocal imaging is a new way invented initially in microscopy [6]. In confocal imaging laser light is tightly focused on an atomic cloud and at any instant, only the illumination volume is imaged. For complete imaging, we need in some way to scan the atomic cloud or the laser light itself. Confocal imaging can be done for absorption and fluorescence imaging. In fluorescence confocal imaging, we can use one objective for both illumination and detection. In addition, the geometry of our cell precludes absorptive confocal imaging. Therefore, in this thesis, we only discuss fluorescence confocal imaging. We use the term whole-field-of-view imaging for any non-confocal type of imaging.

![Confocal, absorption and fluorescence imaging](image)

**Figure 1** Confocal, absorption and fluorescence imaging
In confocal imaging, for the case of atoms in the lattice, the scanning is done by changing the relative phases of lattice beams. In modern confocal microscopes, the laser light is scanned by rotating mirrors or by a high speed acousto-optic deflector instead of scanning the sample itself. Schematics of the typical setup are given in Figure 1.

In the confocal setup, the 405 nm laser light passes through a sub-resel pinhole\(^1\) to constrain the illumination to a diffraction limited point. About 14\% of 767 nm scattered photons will gather at the objective and focus on second pinhole placed at the focal point of the lens (confocal pinhole) to be detected by a single photon detector. The confocal pinhole blocks photons from outside of the focal point and improves the clarity of the final image. The interesting features of this scheme for us are high resolution, and the use of a single photon detector.

The resolution of an objective lens is directly proportional to the wavelength. This means that with the same numerical aperture\(^2\), the resolution of imaging at 405 nm will be about 1.9 times better than the resolution at 767 nm, the wavelength of the D2 line of potassium. In confocal imaging, resolution is determined by the laser wavelength which is 405 nm, however, it can be even slightly better [7].

Detectors like photomultiplier tubes and Avalanche Photo Diodes (APD) can detect even a few photons. Only 14\% of the scattered photons will arrive at the detector. And the wavelength of roughly five-sixths of the photons scattered from the 405 nm excitations, is 767 nm (both these points have been discussed in more detail in section 2.1 ). Therefore, for detection of one 767 nm photon, each atom must scatter a total of about 10 photons. On the other hand, in whole-field-of-view-imaging, the detector is a CCD camera. In the very low photon number regime, the dominant part of the noise comes from the detection unit. For our CCD camera, even to achieve S/N=1, the detection of about 10 photons is needed. This means that roughly each atom should scatter about 60 photons at the desired wavelength. For 405 nm imaging, this means that each atom must scatter about 350 total

---

1. Resel is the radius of the diffraction pattern of a point source.
2. Numerical aperture (N.A.) is the sine of the half angle of the lens acceptance cone and is a measure of the collection efficiency of the objective.
photons, because only 1/6\textsuperscript{th} of the scattered photons are at 405 nm. For 767 nm imaging, the total number of required scatterings for each atom is less, about 60 photons, but at the expense of resolution.

This huge difference will greatly reduce heating in the lattice and therefore, cut down the required lattice depth for confocal imaging. This is even more meaningful if we notice that the 405 nm transition is not a cycling transition.

Finally, it is worth mentioning that whole-field-of-view imaging has an important advantage over confocal imaging. In the former, the entire lattice is being imaged in one shot, so imaging time is independent of the number of lattice sites. In contrast, in confocal imaging, the imaging time is proportional to the number of lattice sites.

### 2.1. 405 nm and 767 nm transitions

\(^{40}\text{K}\) and \(^{6}\text{Li}\) are the only two neutral alkali fermions with stable nuclei. Because of technical issues, working with Potassium is easier and of great interest. A dispenser can be used as a source of Potassium and unlike Lithium, it does not interact with glass. Potassium can sympathetically be cooled with \(^{87}\text{Rb}\). Also, large positive scattering length \(a \approx 10.4\ \text{nm}\) between two species, \(|\frac{9}{2},\frac{9}{2}\rangle\) and \(|\frac{9}{2},\frac{7}{2}\rangle\), implies a strong elastic interaction which allows us to cool it using two spin species [8]. And finally, recoil energy of the D2 line transition for Potassium is 9 times smaller than that for Lithium; therefore with the same lattice depth, Potassium can scatter 9 times more photons. In the following two sections, we will derive the steady state solution of the excited state population of multilevel Potassium atoms, for the case of imaging at 405 nm. Then, we calculate the respective heating rates of 405 nm and 767 nm transitions. The fine level scheme of \(^{40}\text{K}\) is shown in Figure 2 and the related spontaneous emission rates are given in Table 1.
Table 1  scattering rates, wavelengths and recoil frequencies of \(^{40}\)K fine structure transitions

\[
\begin{align*}
\gamma_1 &= 3.82 \times 10^7 \text{ (s}^{-1}) , & \lambda_4 &= 766.7 \text{ nm}, & \omega_{r_1} &= 2\pi \times 7.965 \text{ kHz} \\
\gamma_2 &= 1.24 \times 10^6 \text{ (s}^{-1}) , & \lambda_2 &= 404.5 \text{ nm}, & \omega_{r_2} &= 2\pi \times 28.65 \text{ kHz} \\
\gamma_3 &= 1.4 \times 10^6 \text{ (s}^{-1}) , & \lambda_3 &= 3139.3 \text{ nm}, & \omega_{r_3} &= 2\pi \times 477 \text{ Hz} \\
\gamma_4 &= 4.5 \times 10^6 \text{ (s}^{-1}) , & \lambda_4 &= 2721.2 \text{ nm}, & \omega_{r_4} &= 2\pi \times 637 \text{ Hz} \\
\gamma_5 &= 2.2 \times 10^7 \text{ (s}^{-1}) , & \lambda_5 &= 3160.2 \text{ nm}, & \omega_{r_5} &= 2\pi \times 468 \text{ Hz} \\
\gamma_6 &= 7.9 \times 10^6 \text{ (s}^{-1}) , & \lambda_6 &= 1243.3 \text{ nm}, & \omega_{r_6} &= 2\pi \times 3.02 \text{ kHz} \\
\end{align*}
\]

\(\gamma_i \equiv \gamma_2 + \gamma_3 + \gamma_4\), \(\frac{\gamma_2}{\gamma_i} \sim 1 / 5.76\)

By the use of Einstein coefficients, the following relations can be written down for the rates of transitions within the steady state assumption.

\[
\begin{align*}
5P : & \quad (\gamma_2 + \gamma_3 + \gamma_4)\rho_{5p} = B I (\rho_{4S} - \rho_{5p}) \\
5S : & \quad \gamma_4\rho_{5p} = \gamma_6\rho_{5S} \\
3d : & \quad \gamma_5\rho_{5p} = \gamma_5\rho_{3d} \\
4P : & \quad \gamma_5\rho_{3d} + \gamma_6\rho_{5S} = \gamma_1\rho_{4p} \\
4S : & \quad \gamma_1\rho_{4p} + \gamma_2\rho_{5p} = B I (\rho_{4S} - \rho_{5p}) \\
\end{align*}
\]

Solving these relations, we have

\[
\rho_{5p} = \left( \begin{bmatrix}
\frac{\gamma_3}{\gamma_5} + \frac{\gamma_4}{\gamma_6} + \frac{\gamma_3 + \gamma_4}{\gamma_1} \\
\gamma_5 \\
\gamma_6 \\
\gamma_1 \\
\end{bmatrix} + \frac{\gamma_1}{B I + 2} \right)^{-1},
\]

(2)
where $\gamma_i \equiv \gamma_2 + \gamma_3 + \gamma_4$. We should keep in mind that Einstein coefficients were originally used for black body radiation with the coefficient $B$ containing $g(\omega)$, the frequency distribution of radiation.

In the case of interaction of atom with laser light, in order to find the relevant $B$, the master equations of a 3 level atom were solved and the solution was compared with Einstein coefficient approach in the steady state case.

Consider a three level system as given in Figure 3. The solution from Einstein coefficients is

$$\rho_{sp} = \left(\frac{\gamma_{23}}{\gamma_{13}} + \frac{\gamma_{12} + \gamma_{23}}{B I} + 2\right)^{-1}.$$  \hspace{1cm} (3)

Master equations for a multilevel atomic system are [9]

$$\frac{d\rho}{dt} = \frac{1}{i\hbar} [H, \rho] + \sum_{\epsilon_j \rightarrow \epsilon_i} \gamma_{\epsilon_i \epsilon_j} L_{ji} \rho,$$

$$L_{ij}\rho = \frac{1}{2} (2\sigma_{ji} \rho \sigma_{ji} - \sigma_{ji} \rho - \rho \sigma_{ji}), \quad \sigma_{ij} = |i\rangle\langle j|,$$  \hspace{1cm} (4)

where the sum is over all transitions from excited states to ground states. In the case of light resonant with the transition between levels 1 and 2, $H$ is given by
\[ H = \frac{i}{2} \begin{pmatrix} 0 & \Omega e^{ikz} & 0 \\ \Omega^* e^{-ikz} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \] (5)

\( \Omega \) is the Rabi frequency and can be written in a simple form

\[ \Omega = \gamma_{12} \sqrt{\frac{I}{2I_s}} \quad (I_s = \frac{2\pi^2 \hbar c \gamma'_{12}}{3\lambda_{12}^3}). \] (6)

The steady state solution of these master equations results in

\[ \rho_{23} = \left( \gamma'_{23} + \frac{(\gamma_{12} + \gamma_{23})^2}{|\Omega|^2} + 2 \right)^{-1}. \] (7)

From comparing this solution to the solution of Einstein rate equations, we are able to read off the coefficient \( B \) as

\[ B = \frac{\gamma_{12}}{2I_s} \frac{\gamma_{12}}{\gamma_{12} + \gamma_{23}}. \] (8)

For the original problem of a 5 level atomic system, with the substitution of

\[ \gamma_{12} \rightarrow \gamma_2 \]
\[ \gamma_{12} + \gamma_{23} \rightarrow \gamma_t \]
\[ \gamma_{13} \rightarrow \gamma_1, \]

we achieve

\[ \rho_{SP} = \left( \gamma_5 + \gamma_6 + \gamma_3 + \gamma_4 \gamma_1 + \frac{\gamma_2^2 2I_{4S\rightarrow 5P}}{I} + 2 \right)^{-1}, \] (10)

where

\[ I_{4S\rightarrow 5P} = 3.7 \text{ W/m}^2, \]

\[ \frac{\gamma_3 + \gamma_4 + \gamma_3 + \gamma_3}{\gamma_5 + \gamma_6 + \gamma_1} = 0.79, \] (11)

\[ \frac{\gamma_2^2 2I_{4S\rightarrow 5P}}{\gamma_2^2 I} = 245 / I. \]

When \( I < I_s \), we can estimate the population to be

\[ \rho_{SP} = \frac{\gamma_2^2 I}{\gamma_t^2 2I_{4S\rightarrow 5P}}. \] (12)

For on-resonance 767 nm imaging, the steady state population of the excited state (4P) is easily given by the solution of the master equations for two level atoms.
\[ \rho_{4p} = \frac{\Omega^2}{4\delta^2 + 2\Omega^2 + \gamma_1^2} \approx \frac{1}{2} \frac{I}{I_{4S\rightarrow4P}}, \]  

(13)

where \( \delta \) is the detuning and resonance has been assumed in the second equality. Saturation intensity of the \( 4S \rightarrow 4P \) transition is

\[ I_{4S\rightarrow4P} = 16.7 \text{ W/m}^2. \]  

(14)

The scattering rates at 767 nm and 405 nm, for fluorescence whole-field-of-view-imaging, are \( \gamma_1 \rho_{4p} \) and \( \gamma_2 \rho_{5p} \). The respective desired intensity of imaging beams, for the same number of scattered photon at desired wavelengths and for the same imaging time, is

\[ \frac{I_{405}}{I_{767}} = \frac{\gamma_1 I_{4S\rightarrow5P}}{\gamma_2 I_{4S\rightarrow4P}} \approx 225. \]  

(15)

This relative high intensity for 405 nm will cause extra heating due to rescattering in the lattice and also increase the noise level in the detector due to absorption and reemission in the imaging window and objective. Also, in the case of whole-field-of-view imaging at 767 nm, the wavelength of all scattered photons is 767 nm. In contrast, for the imaging at 405 nm, only \( \frac{\gamma_2}{\gamma_1} \approx \frac{1}{5.76} \) ths of the scattered photons have the desired wavelength of 405 nm. If we assume that N.A. = 0.75, roughly about 14% of the scattered photons will be gathered by the objective. In fluorescence imaging, for detection of each photon at 405 nm, atom must scatter about 8 photons at 405 nm; which means that in order to detect a single photon in the CCD, one atom must scatter a total of about 46 photons. In confocal imaging, \( \frac{\gamma_1 - \gamma_2}{\gamma_1} \approx 83\% \) percent of scattered photons will have the desired wavelength of 767 nm. These numbers clearly show that the improvement in resolution obtained from whole-field-of-view imaging at 405 nm, is inevitably accompanied by further complications and restrictions.
2.2. Heating rate in the lattice

Before talking about heating in the lattice, it is useful to derive average heating due to a single scattering cycle for both 767 nm and 405 nm transitions. At this moment, we will neglect rescattering events. Consider a simple two level atom with momentum $p$ which absorbs a photon with a $\vec{k}$ vector along $z$ axis. The total change of momentum after scattering is given by

$$\Delta p = (-\hbar k \sin \theta \cos \phi, -\hbar k \sin \theta \sin \phi, \hbar k - \hbar k \cos \theta),$$

where $\theta$ and $\phi$ are azimuthal angles of the scattered photon. The average increase in energy per scattering cycle, is derived by integrating over the whole solid angle

$$\Delta E_{\text{avg}} = \frac{\Delta p_x^2 + \Delta p_y^2 + \Delta p_z^2}{2m} = \frac{E_R}{3} + \frac{E_R}{3} + \frac{4E_R}{3} = 2E_R. \quad (17)$$

Here $E_R$ is the recoil energy. Spontaneous emission is responsible for heating by $E_R/3$ for each spatial degree of freedom. Another $E_R$ arises from absorption of a photon. In the 5 level scheme of the 405 nm transition, each scattering is a combination of 6 fluorescence events with different wavelengths. In the steady state situation, heating rate can be written as

$$\text{Heating rate} = \text{rate of scattering} \times E_{R,2} + \sum_i \text{rate of spon. level}(i) \times E_{R,i},$$

$$= (\gamma_2 + \gamma_3 + \gamma_4)\rho_{5p}E_{R,2} + E_{R,2}\gamma_2\rho_{5p} + E_{R,3}\gamma_3\rho_{5p} + E_{R,4}\gamma_4\rho_{5p} + E_{R,5}\gamma_5\rho_{3d} + E_{R,6}\gamma_6\rho_{5s} + E_{R,1}\gamma_1\rho_{4p}, \quad (18)$$

where $i$ is the index of transitions which are given in Figure 2 and $E_{R,1} = E_R$. After dividing heating rate by the rate of scattering, heating due to each scattering event is obtained

$$\Delta E_{\text{avg}} = E_{R,2}(1 + \gamma_2 / \gamma_i) + (E_{R,3} + E_{R,5})\gamma_3 / \gamma_i + (E_{R,4} + E_{R,6})\gamma_4 / \gamma_i$$

$$+ E_{R,1}(\gamma_1 + \gamma_4) / \gamma_i \approx 4.24 E_R. \quad (19)$$

The first equality has been written by using relations (1). This result shows that scattering of a 405 nm photon heats the atom about 2 times more than the scattering of a 767 nm photon.
Heating due to rescattering and its role in the lattice is more complicated. In [10], S. Wolf et al. have addressed this issue in their experiments. One of their interesting results is the linear time dependence of heating both in the lattice and in the dense cloud of free atoms. We will use this assumption in the rest of this thesis.

In a deep lattice, they have shown that when $\gamma_s / \omega_0 \ll 1$ ($\gamma_s$ is the spontaneous scattering rate and $\omega_0$ is the lattice frequency), rescattering heating is suppressed and the overall heating rate in the lattice is roughly equal to the heating rate for a single free atom. In our lattice, to achieve single atom imaging, we desire to have only one or two lattice planes; therefore rescattering heating will be absent even at high intensities.

\subsection{2.2.1. Optical density}

Optical density due to a single atom in a lattice with unity filling, is given by

$$OD = 1 - \frac{\text{# of scattered photons}}{\text{# of incident photons}} = 1 - \frac{\gamma_0 T}{I_0 T d_{\text{lattice}}^2 / h\omega_{\text{imaging}}},$$

(20)

where $d_{\text{lattice}}$ is the spatial period of the lattice. For $d_{\text{lattice}} = 700 \mu m$, using equations (12) and (13) will result in

$$OD_{767} = 0.57, \quad OD_{405} = 0.005.$$

(21)

Therefore in the case of 767 nm fluorescence whole-field-of-view imaging, because of the side illumination, even a one layer lattice will be optically thick; therefore we need off-resonant light and consequently, longer imaging time.

\subsection{2.3. Optical resolution}

Point spread function (PSF) of a lens is the intensity distribution that results from a point self-luminous object. In the paraxial approximation, the diffraction pattern of a circular aperture at the focal plane is given by
\[ P(0, \rho) = I_0 \left( \frac{2J_1(\rho)}{\rho} \right)^2, \]  

(22)

where \( \rho = r k NA \) is the lateral optical unit and \( J_1 \) is the Bessel function of the first kind \[11\]. The first dark ring occurs at \( \rho = 1.22 \pi \) and is called the first Airy disk. The Radius of the point spread function is a “resel”

\[ r_{PSF} = \frac{1.22 \lambda}{2 N.A.}. \]  

(23)

According to the Rayleigh criterion, two objects are optically resolved if they are separated by a resel. For the case of circular aperture, the Rayleigh criterion is reached at a saddle point at the intensity of about 0.74 times of the maximum intensity or CTF=0.15 (Figure 4). Intensity of the dip, in the case of rectangular aperture, is about 0.81 times of the maximum and CTF=0.10. Some people define the resolution as the FWHM of the Airy disk which is about 0.84 \( r_{PSF} \).

In fact, the correct definition of the resolution is application-dependent and strongly tied to the noise level of the image. In our case, the number of detected photons for each atom can be very small (about 10 photons) and the photon shot noise alone is about 30% of the signal. Therefore, the Rayleigh criterion is an under-estimation. In contrast, in optical microscopes, as the number of detected photons for each pixel of CCD camera is around \( 10^{10} \), we can resolve two points even with a dip of a few percent. In this part, we will continue with the Rayleigh definition of resolution to point out important issues.
Along the optical axis the point spread function is given by

\[ P(\zeta,0) = I_0 \left( \frac{\sin(\zeta/4)}{\zeta/4} \right)^2, \]  

(24)

Where \( \zeta = k z NA^2 \) is the axial optical unit. The first node occurs at

\[ z_{PSF} = \frac{2\lambda}{N.A.}. \]

(25)

The depth of focus usually is defined as the amount of axial displacement that doubles the apparent diameter of the Airy pattern. It is given by

\[ \Delta z = \frac{\lambda}{2N.A.}. \]

(26)

In equation (24), the point spread function is only considered at the focal point; however, it can be defined for any parallel optical plane. The integral of PSF on all of these planes is constant and equal, because, according to the initial definition, PSF is the distribution of intensity. So, it is important to notice that \( Z_{PSF} \) does not define any useful axial resolution for our optical lattice. In fact, atoms in farther lattice planes with even \( z = 100\Delta z \), can make a blurry image in the detector and therefore decrease the contrast of the image. True axial resolution is achievable in confocal imaging [7].

In confocal imaging, the overall PSF is given by product of illumination PSF \( (P_s) \) and the objective PSF \( (P_d) \), which is given by equation (22) [7]

\[ P_{conf}(\rho,\zeta) = P_s(\rho,\zeta) \cdot P_d(\rho,\zeta). \]

(27)

The reason is that PSF is the diffraction pattern of the opening aperture of the objective. Therefore, it is a property of the lens and does not depend on the object. In case of identical illumination and detection, when two PSFs are the same, resolution from the Rayleigh criterion of 26% is given by

\[ r_{conf} = 0.72 \text{ resel} = \frac{0.88\lambda}{2N.A.}. \]

(28)

In our confocal configuration, the wavelength of laser light and detected photons are different. The Rayleigh resolution is a bit better than resel size of the laser light which has
a narrower PSF ( $r_{\text{conf}} \approx r_{\text{PSF}}^{405} = 330 \text{ nm}$ ). Although the resolution in confocal imaging is a bit better than whole-field-of-view imaging, the more important difference between these two is the vanishing of side peaks in the axial PSF of confocal imaging. Because of the pinhole in the detection, integral of the PSF of confocal imaging is not the same for planes parallel to the focal plane. In this case, we have a real axial resolution which is typically given by

$$\Delta z_{\text{conf}} = \frac{1.5\lambda}{N.A.^2}. \quad (29)$$

As can be seen, the role of the detection pinhole is very important in confocal imaging. However, a pinhole smaller than resel only decreases the number of photons reaching the detector and does not enhance resolution. In contrast, a wide pinhole can not block photons from outside of the focal volume. As a compromise, the proper diameter of the pinhole is about 3 resels which is about 100 $\mu$m for a $50\times/0.7$ objective at 767 nm.

The paraxial assumption underlies the derivation of these relations, but is hardly correct for high N.A. However for high N.A. lenses, the width of the point spread function is only a bit greater than this result[7]. Under paraxial approximation, a more precise relation for resolution of infinitely corrected objectives is given in[12], however that is only correct for small N.A.

### 2.3.1. Pixellation effect

The pixellation effect is another issue in resolution which applies in whole-field-of-view imaging where we use CCD camera. From Nyquist sampling theory, the frequency of sampling must be greater than twice of the maximum frequency of the image. The highest frequency of the image is determined by the diffraction limit of the optics, therefore the pixel size must be

$$\text{pixel size} \leq \frac{r_{\text{PSF}}}{2.3}.$$  \quad (30)

Here, 2.3, in place of 2, is an empirical value[13]. Because of the weakness of our photon signal, we take the above as an equality. For the PIXIS 1024 camera from
Princeton instruments that we are now using in our lab, each pixel size is 13 μm. For a 40X objective lens and lattice spacing 700 nm, this equality is already nearly established. Figure 5 shows the effect of pixellation on contrast. MTF is calculated by averaging over many periods. The sudden drop is at the Nyquist limit and corresponds to the situation where each atom is placed between two pixels and therefore all the pixels have the same amplitude. As it is shown, by using a higher magnification, improvement of pixellation MTF is possible. However, the cost incurred will be lesser photon number per pixel. The condition stated in equation (30) is equivalent to MTF>0.51 for pixellation. According to Nyquist theory, the curve is meaningless beyond the Nyquist limit.

![MTF graph](image)

**Figure 5** Pixellation MTF for a 40x objective. The vertical line is just at the Nyquist limit for pixel size of 13 μmx13 μm.

### 2.4. Experimental reports

Recently, Sortais et al. reported an experiment on single $^{87}$Rb atom trapped in an optical trap of a few microns[14]. In this experiment, confocal fluorescence detection has been used with high numerical aperture optics. They employed two kinds of detectors: APD and CCD cameras. A commercial large numerical aperture (N.A.=0.5) aspheric lens was put inside the vacuum and a few standard lenses outside. Their objective was infinity-corrected and diffraction limited at 780 nm. They also trapped two single atoms in two dipole traps of 1 μm diameter separated by 2.2 μm, and imaged them with a CCD camera of 13 μm×13 μm pixel size. The overall transverse magnification of their
imaging system is ~ 25 and therefore it images their 1 \( \mu m \) diameter dipole trap onto a 2 pixel \( \times \) 2 pixel area. Figure 6 shows a cross section of their CCD image when both traps were loaded with single atoms. The width of the Gaussian fits to the peak signal of each atom is 0.9 \( \pm \) 0.2 \( \mu m \), which is close to the theoretical resolution of 0.84 \( \times \) \( \frac{1.22 \times 780}{2 \times 0.5} \) \( \approx \) 0.8 \( \mu m \). This shows that they are able to resolve atoms separated by more than two resels (2 \( \mu m \)).

Figure 6 Cross-section of a CCD image showing two single atoms trapped in two adjacent optical tweezers, corrected for the magnification (\( \times 25 \)) of the imaging system. The distance between the two optical tweezers is 2.2\( \pm \)0.1 \( \mu m \). Each peak is fitted by a gaussian model (dashed lines) and exhibits a waist \( w = 0.9 \pm 0.2 \, \mu m \). The solid line represents the sum of the fits of the two fluorescence signals emitted by each single atom. Vertical bars represent the intensity measured by each pixel of the CCD camera during a time window of 100 ms (figure 7 in [14]).

2.5. Optical Lattice

An optical lattice is a periodic light shift potential produced by interference of two or more counter propagating light beams. In this section, we discuss the lattice depth and its relation with Néel temperature. In order to compare the feasibility of different kinds of imaging, we fix laser power and compare lattice depth and photon number required to achieve less than 1\% error in detection. To produce a 3D lattice with 1 W laser power, we take 300 mW for each direction; in total, six 300 mW laser beams. Light shift due to a Gaussian beam is given by [15]
\[ U_0 \approx \frac{2P}{\pi w_0^2} \left( \frac{3 \pi c^2}{2 \omega_0^2} \left( \frac{\gamma}{\omega_a - \omega_i} + \frac{\gamma}{\omega_a + \omega_i} \right) \right), \]  \hspace{1cm} (31)

where \( P \) is the laser power, \( w_0 \) is the beam waist and \( \omega_a \) and \( \omega_i \) are atom transition and laser frequency. For two counter propagating and linearly polarized lattice beams with the relative angle of polarization \( \theta \), lattice depth is\[ U_p = \left[ \frac{4}{3} U_0 \sqrt{4 \cos^2 \theta + \left( \frac{m}{F} \right)^2 \sin^2 \theta} \right]. \hspace{1cm} (32)\]

For simplicity by considering \( m=F \) and \( \theta = 0 \), lattice depth is
\[ U_p = \frac{8}{3} U_0. \hspace{1cm} (33)\]

For counter propagating beams, lattice spacing is \( \lambda_i / 2 \). According to section 2.3 and 2.6, for high resolution imaging we need to increase lattice spacing. This can be done by changing the angle between the beams. The lattice spacing for two beams with angle \( \varphi \) between them is
\[ d = \frac{\lambda_i}{2 \sin(\varphi/2)}. \hspace{1cm} (34)\]

When the polarizations of both beams are the same and perpendicular to the plane of the beams, lattice depth is independent of \( \varphi \). However, in general situation, lattice depth depends on both the angle between polarizations (\( \theta \)) and that between beams (\( \varphi \)) [17].

Figure 7a shows scattering rate of a single 300 mW beam with \( w_0 = 80 \mu m \) versus detuning of the lattice light. In a 3D lattice, atoms scatter photons from all 6 beams. However, as atoms are placed in low intensity sites of the lattice, scattering rate will be reduced. Figure 7b and c display depth of the lattice (equation (33)) and the lattice wavelength versus detuning of the lattice.
Typically, the scattering rate of the lattice beam is much less than the scattering rate of the imaging beam. Therefore, the noise due to scattering of a lattice beam is negligible.

### 2.5.1. Néel temperature

For temperatures sufficiently low so that atoms are restricted to the first energy band, Hubbard model describes physics of quantum particles in the lattice potential. In this model, the two relevant energy scales are on-site interaction energy ($U$) and tunneling strength ($J$). These two energy scales can be calculated from lattice depth ($V_0$), scattering length ($a_s$) and recoil energy [19]
where $d$ is the lattice spacing. The Hubbard Hamiltonian of a half-filled lattice of two spin species (one atom per site), for energies much smaller than the gap in density excitations ($\sim U$ at large $U$), reduces to quantum Heisenberg model with exchange strength \[20\].

$$J_{AF} = 4J^2 / U. \quad (36)$$

This model, at very low temperature, predicts a paramagnetic-antiferromagnetic phase transition. This critical temperature is called Néel temperature.

In low coupling strength (small $U/J$), the Néel temperature is exponentially small. In the high coupling limit,

$$T_N / J \approx 4J / U. \quad (37)$$

Between these two limits, $T_N/J$ reaches a maximum \[20\]. $T_N/J$ versus $U/J$ is analytically calculated in \[21\] and it is shown that for $U/J\sim 10$, $T_N/J$ is maximum.

In order to display phase transition curves in $(T_N, V_0)$ plane instead of $(T_N/J, U/J)$ plane, we have used the relations for $U$ and $J$ given above. Figure 8 shows this plane mapping for different scattering lengths. Both axes are normalized by recoil energy. The lowest curve can be found in \[22\]. Werner et al. \[23\] have shown that at $U/J=10$, the one-band Hubbard model is valid for $a_s<0.02 \lambda/2$. In $^{40}$K, the $|9/2, 9/2\rangle$ magnetic state is a low field seeker and will be used for trapping and cooling. However, the scattering length between $|9/2, 9/2\rangle$ and $|9/2, 7/2\rangle$ states is 196 Bohr radii \[8\], which is equivalent to $0.027 \lambda/2$. Therefore, in order to achieve the antiferromagnetic phase with these states, using Feshbach resonance is a must. Scattering length between $|9/2, -9/2\rangle$ and
\( |9/2,-7/2\rangle \) states is 104 Bohr radii \([24]\) or \(0.014 \lambda/2\). The curve corresponds to this scattering length is shown in Figure 8 by a thicker line. After cooling the \( |9/2,9/2\rangle \) magnetic state, we will transfer atoms to \( |9/2,-9/2\rangle \) and \( |9/2,-7/2\rangle \) states. Then, by further evaporation in the absence of Feshbach resonance, we will be able to reach Néel temperature. For a lattice depth of \(7E_R\), in the absence of Feshbach resonance, Néel temperature is given by

\[
T_N \sim 0.015 E_R. \tag{38}
\]

Néel temperature is a few nano-Kelvins and is inversely proportional to the square of the lattice spacing. Therefore, for single atom imaging, it is desirable to decrease the lattice spacing.

![Figure 8](image)

**Figure 8** Néel temperature versus lattice depth for different scattering lengths. The shown scattering lengths are from \(0.002 \lambda/2\) to \(0.02 \lambda/2\) in \(0.002 \lambda/2\) steps, where \(\lambda\) is the lattice wavelength (~765 nm). The thicker curve corresponds to the natural scattering length of \(a_s \sim 104\) Bohr radii between \(|9/2,-9/2\rangle\) and \(|9/2,-7/2\rangle\) magnetic states.

After cooling atoms below \(T_N\), we will increase the lattice depth to hundreds of \(E_R\) (full power) for imaging. Before the imaging cycle, the atoms stay in the antiferromagnetic phase for about the spin exchange time. Spin exchange time in the Heisenberg exchange Hamiltonian is given by the Heisenberg time
\[ t_h = \frac{\hbar}{J_{AF}} \sim \frac{\hbar}{0.02E_R} \quad (for\ V_0 = 7E_R). \]  

(39)

For efficient cooling below the Néel temperature (T_N), we require the heating due to lattice beam scattering to be much less than the Néel temperature.

\[ \gamma_n(2E_R)t_h << 0.015E_R. \]  

(40)

Table 2 shows the requirements for lattice beam heating to be one tenth of the Néel temperature for \( V_{lattice} = 7E_R^{scaled} \). The difference between 405 nm and 767 nm imaging is only in their resel size. The last column shows the maximum photon number that an atom can scatter before reaching the lattice height. Scattering of a 767 nm photon will heat an atom by \( 2E_R \) and scattering of a 405 nm photon will heat an atom by \( 4.24E_R \). In these calculations, the intensity of each lattice beam is 300 mW and beam waist is 100 \( \mu m \). In the third column, resel is for N.A. = 0.7.

Table 2  lattice requirements and parameters to achieve Néel temperature and take an image.

<table>
<thead>
<tr>
<th>Imaging</th>
<th>( \delta_{lattice}/\gamma_1 )</th>
<th>d/resel</th>
<th>d (nm)</th>
<th>( T_N ) (nK)</th>
<th>( V_{lattice}/E_R ) (full depth)</th>
<th>Max. Photon number</th>
</tr>
</thead>
<tbody>
<tr>
<td>at 767 nm</td>
<td>( 1.2 \times 10^6 )</td>
<td>1.5</td>
<td>1003</td>
<td>0.80</td>
<td>246</td>
<td>123</td>
</tr>
<tr>
<td></td>
<td>( 2.1 \times 10^6 )</td>
<td>2</td>
<td>1337</td>
<td>0.45</td>
<td>137</td>
<td>68</td>
</tr>
<tr>
<td>at 405 nm or confocal</td>
<td>( 3.4 \times 10^5 )</td>
<td>1.5</td>
<td>529</td>
<td>2.77</td>
<td>849</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>( 6.1 \times 10^5 )</td>
<td>2</td>
<td>705</td>
<td>1.57</td>
<td>481</td>
<td>113</td>
</tr>
</tbody>
</table>

2.6. S/N and required photon number

According to the discussed experiment, the atom separation (or lattice constant) of about two resels is appropriate. Because of the weakness of the imaging signal, we like to work close to the Nyquist limit. This separation is equivalent to a pixel size of one resel at the Nyquist limit. For confocal and whole-field-of-view imaging at 405 nm by an objective lens with N.A. = 0.75, the Rayleigh resolution is \( r_{rad} = 330 \mu m \). For instance, let us take lattice spacing to be \( d \approx 700 \mu m \), which is a bit more than two resels. This separation
with magnification 40X and pixel size $13\,\mu m$, already satisfies equation (30). Smaller lattice spacing is possible but to keep equation (30) true, we need higher magnification. For whole-field-of-view imaging at 767 nm, the Rayleigh resolution is $r_{PSD} = 624\,nm$.

For $d \approx 700\,\mu m$ and fluorescence imaging at 767 nm, the height of the saddle point is 52.6% of the maximum. With 60% reduction of the CTF due to pixellation for hypothetical noiseless detection, the best possible CTF is 12%, which corresponds to a 78% saddle height. Figure 9 displays the probability of correct detection of a saddle point versus the ratio of the depth of the saddle point ($\Delta \equiv I_{\text{max}} - I_{\text{min}} / I_{\text{max}}$) to the standard deviation of the noise. For a 99% correct detection, $\Delta / \sigma_{\text{noise}} \sim 3.1$. For the calculation, we have used Gaussian approximation for the noise distribution.

![Figure 9](image.png)

**Figure 9** probability of correct detection of saddle point versus ratio of the saddle depth to noise standard deviation. It is assumed that imaging is at the Nyquist limit and applied pixellation effect MTF=0.40 is for this limit. The circle shows the point of correct detection of 99%.

For 99% correct detection, noise amplitude must be less than $22/3.1=7.1\%$ of the signal or equivalently S/N$>14.1$. When the noise is shot noise limited, for a pixel to resolve an atom, it needs to detect about 288 photons. With a quantum efficiency of 80% and a collection efficiency 14% (N.A.=0.70), each atom must scatter more than 1775 photons.

This simple reasoning can be extended to 2D lattices where the interference from neighboring atoms will further decrease the contrast. The case of absorption imaging is a
bit more complicated. In absorption imaging, signal is the reduction in laser light and is directly proportional to optical density. Figure 10 shows the required number of scatterings by each atom in order to achieve less than 1% detection error. For the calculations, we assumed that quantum detection efficiency of CCD at 767 nm (405 nm) is 0.8 (0.6) and quantum detection efficiency of the single photon detector is 50%.

Figure 10  Required number of scatterings by each atom in order to achieve less than 0.01 detection error. Curves corresponding to fluorescence and absorption at 405 nm are sub-scaled by the factors given on them. The circles show the maximum allowed scattered photon number given in Table 2. The curves are calculated for N.A.=0.7 and for all points, the Nyquist limit is assumed.

When the lattice spacing approaches one resel, interference among diffraction patterns of single atoms grows fast. Interference reduces the contrast and increases the required photon number for a fixed detection error. In the figure, this effect is displayed by the sharp rising slopes of the curves in low lattice spacing close to a resel. In absorption imaging, on increasing the lattice spacing, optical density, and therefore contrast, decrease. For this reason absorption curves start to increase at a lattice spacing of about
1.6 resels. The slight increase in fluorescence curves after two resels spacing is due to interference of second order fringes.

The circles in this figure show the maximum possible photon number given in Table 2. For parameters for which the data of Table 2 have been calculated, according to the figure, absorption imaging at 767 nm, with lattice spacing greater than 880 nm, is the only possible imaging scheme. Confocal imaging is just on the border for both 1.5 and 2 resel spacing, as shown in the figure. Fluorescence imaging at 767 nm is off by more than a factor of 4. Absorptive and fluorescence imaging at 405 nm are quite impossible.

In Table 2, we assumed $w_0 = 100 \mu m$ and $P = 300$ mW. By increasing the laser power or decreasing beam waist of the lattice beams, it is possible to increase the maximum allowed photon number. With this increase, even fluorescence imaging at 767 nm, besides absorption imaging at 767 nm and confocal imaging, can be possible. However, compared with fluorescence imaging, for the small spacing that we are especially interested in, absorption imaging is far superior. One of the main differences between absorption and fluorescence imaging is in the collection efficiency which makes the absorptive signal about 7 times greater. For absorption imaging at 405 nm where optical density, and hence absorptive signal, is very small, fluorescence imaging is better, although both of them are impossible.

Table 3 summarizes the main results of this chapter. Parts of fourth and sixth columns are from Table 2. Gray cells indicate that imaging is impossible. In order to be able to image atoms, maximum allowed photon number must be greater than needed photon number. For imaging time, we assumed that for absorption imaging, population of excited state is 1/10 and for fluorescence, is 1/2. In absorption, further increasing the population will saturate atoms and decrease optical density, thereby increasing noise. In confocal imaging, from equation (10), the maximum population of excited state is 1/2.79. We scan a 10x10 optical lattice.
Table 3  Compression of imaging methods.

<table>
<thead>
<tr>
<th>Imaging method</th>
<th>d (nm)</th>
<th>Needed ph. #</th>
<th>Max. ph. #</th>
<th>Imaging time (µs)</th>
<th>T_N (nK)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>(w_0 = 100 µm)</td>
<td>(w_0 = 60 µm)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Confocal</td>
<td>529</td>
<td>217</td>
<td>200</td>
<td>556</td>
<td>8598</td>
</tr>
<tr>
<td></td>
<td>705</td>
<td>115</td>
<td>113</td>
<td>321</td>
<td>4557</td>
</tr>
<tr>
<td>Absorption 767 nm</td>
<td>1003</td>
<td>33</td>
<td>123</td>
<td>342</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td>1337</td>
<td>58</td>
<td>68</td>
<td>192</td>
<td>17</td>
</tr>
<tr>
<td>Fluorescence 767 nm</td>
<td>1003</td>
<td>616</td>
<td>123</td>
<td>342</td>
<td>35</td>
</tr>
<tr>
<td></td>
<td>1337</td>
<td>328</td>
<td>68</td>
<td>192</td>
<td>19</td>
</tr>
</tbody>
</table>
3. Imaging window

Designing an aberration corrected objective is hard work, so we prefer to use commercial microscope objectives available in the market. Microscope objectives are not vacuum compatible. For this reason we would like to place all of our imaging systems outside the vacuum chamber. Therefore, we need to use objectives designed to work with a coverslip, which is a glass strip that we will use as a vacuum window. Standard coverslips are made from fused quartz and their standard thickness is $170 \mu m$. However, a $170 \mu m$ thick fused quartz coverslip cannot withstand atmospheric pressure. We should also keep in mind that spherical aberration is proportional to the thickness of the coverslip. Numerical aperture is the sine of the half angle of the imaging cone and is a measure of the light collection efficiency of objectives. With high numerical aperture (N.A.) objectives, the aberration is more sensitive to the thickness. For compensation of thickness deviation in coverslips, optical companies have designed objectives with correction collars. A correction collar is a ring that can adjust the distance between lenses in the objective to work with a range of coverslip thicknesses. Dry objectives with N.A.$>0.9$ can work with coverslip thickness in the range $0.11-0.23$ mm. Objectives with lower N.A. can be used for up to $2$ mm.

This chapter deals with requirements that our imaging window must satisfy to keep the imaging system diffraction limited. Sapphire and fused quartz have been chosen for evaluation. Fused quartz is standard material for coverslip; however it is not possible to use it for N.A.$>0.9$ objectives and vacuum window at the same time. Sapphire is not standard coverslip material and therefore, produces some aberration. However, its higher stiffness allows a much thinner window to be used. The main effects that restrict possible thicknesses of the optical window are rupture, bending due to differential pressure, birefringence effect in crystals, induced birefringence due to stress, and mismatch of the indices of refraction. In this chapter, we will discuss these effects and the resultant restrictions on sapphire and quartz windows. In

1. Numerical aperture is the sine of the half angle of the imaging cone and is a measure of the light collection efficiency of objectives.
[25], it is showed that the effect of induced birefringence due to stress is negligible, therefore we will not discuss this issue.

3.1. Sapphire and fused quartz

Sapphire is one of the hardest materials in nature and makes the hardest optical windows after diamond. Sapphire with different crystal orientations is available commercially, in various surface qualities and as thin as few tens of microns. It has a high transmission range with transmission of about 84% from ultraviolet to mid IR. However, there are some difficulties in its usage for high resolution imaging. Birefringence is a major issue. Also, the difference in index of refraction compared to fused quartz may cause problems.

On the other hand, fused quartz is the ideal optical window. It can be easily found in different thicknesses and sizes due to its widespread applications in microscope slides and coverslips. It has high transmission range with the transmittance >90% in the visible range and near IR spectrum. However due to its lower stiffness, we can not use it for very high numerical aperture objectives. In Table 4, some properties of sapphire and quartz are given.

| Table 4  Mechanical, optical and thermal properties of sapphire and fused quartz. |
|---------------------------------|-----------------|-----------------|
| **Mechanical properties**       | Unit            | Sapphire        | Fused Quartz    |
| Modulus of rupture (MOR)        | MPa             | 442-680         | 50              |
| Young modulus                   | GPa             | >335            | 73              |
| (Modulus of elasticity)         |                 |                 |                 |
| **Optical properties**          |                 |                 |                 |
| Refraction index at 405 nm      | O: 1.785        |                 | 1.470           |
|                                 | E: 1.705        |                 |                 |
| Refraction index at 767 nm      | O: 1.761        |                 | 1.455           |
|                                 | E: 1.754        |                 |                 |
| **Thermal properties**          |                 |                 |                 |
| Coefficient of thermal expansion| cm/cm.ºC x10⁻⁶  | 7.7 ⊥ c-axis    | 0.59            |
3.2. **Strehl ratio and Marechal criterion**

The term aberration is used to denote any distortion in the wavefront of a beam from the ideal wavefront. For example, in our confocal imaging, we use two colors of light. It is possible that their focal lengths are different and that one of them becomes off-focus. Thus, their wavefronts will have a relative phase shift and the optics will suffer from chromatic aberration. The definition of resolution of a lens that we have used is applicable for aberration corrected optics. Existence of any aberration will degrade imaging quality and decrease resolution. To quantify aberration, the relation of optical path difference in the wavefront and diffraction intensity has been explored in literature\[26\]. The Optical Path Difference (OPD) in question is the optical path difference between aberrated and non aberrated wavefront.

Strehl ratio (SR) is defined as the ratio of the intensity at the centre of the diffraction pattern to that obtained in the aberration free case. It is a measure of aberration in optics. The Strehl ratio is given by

\[
\text{Strehl ratio} = \frac{1}{\pi^2} \left| \int_{0}^{2\pi} \int_{0}^{1} e^{i2\pi \Delta W(\rho, \theta)} \rho d\rho d\theta \right|^2 ,
\]

(41)

where \( \rho \) is the optical unit and \( \Delta W \) is the optical path deference \[27\]. For small aberrations (SR\(>0.5\)) it can be further simplified to

\[
\text{Strehl ratio} \approx \left[ 1 + (2\pi)^2 \left[ \frac{\Delta W^2}{2^2} - \overline{\Delta W^2} \right] \right]^2 \approx 1 - \left( \frac{2\pi\sigma}{\lambda} \right)^2 ,
\]

(42)

where \( \sigma \) is the standard deviation of OPD over the wavefront.

Quality of an optical system is determined by Marechal criterion which states that an optical system is corrected for aberration if SR\(>0.8\). This condition is equivalent to \( \sigma < \lambda / 14 \).
3.3. Rupture

The minimum thickness required for a window with fixed edges to withstand a pressure is given by

\[ t = 0.433 \left( \frac{P}{M} \right)^{1/2} D, \]

where \( P \) is the pressure, \( M \) is the modulus of rupture, \( D \) is the diameter[1]. MOR is directly related to surface quality, fabrication process and in the case of sapphire, angle between c-axis and surface of the window. However, datasheets usually contain typical values. Depending on the kind of application, people use thicker windows with different safety factors [25]. Figure 11 shows the required thicknesses of the sapphire and fused quartz windows versus the diameter of the window. Two lines have been drawn corresponding to the minimum and maximum reported MOR for sapphire.

![Figure 11](image_url)  
*Figure 11  Required thicknesses for sapphire and fused quartz to withstand 1 atmosphere pressure*

We have also performed rupture experiments for circular and square sapphire windows with \( t=0.19 \) mm and 0.25 mm. Crosses in Figure 11 show the tests on circular windows. In these tests, the windows were placed on o-rings with different diameters and the edges were not fixed. The circle in the figure corresponds to a test in which a window was glued to a square aluminum frame with 25 mm side size. During the tests, windows were
knocked with the tip of a screw to make sure that they can withstand possible contacts with the objective head. For both thicknesses, we never observed ruptures. In this experiment, pressure in the vacuum side was 0.004 atmospheres.

3.4. **Bending**

A pressure difference will bend the window. A bent window causes a phase shift between the rays with different incident angles on the window. Also, rays at different incident angles are laterally displaced by different amounts. So, in the net result, the converging points for different angles are different. For a flat window also, the converging point depends on the angle but objectives compensate for this effect. Bending puts a restriction on minimum thickness.

Maximum deflection of a square plate is given by

\[ y_m = k \frac{p L^4}{E t^3}, \]

where \( p \) is the pressure, \( L \) is the side, \( E \) is the modulus of elasticity, \( t \) is the thickness and \( k \) is a constant depending on the type of supports at the edges. For a plate fixed at all edges, \( k=0.0138 \) [28]. This equation is valid for \( y_m < 0.4t \).

![Diagram of bent window](image)

**Figure 12** Bended window has been approximated by an arc of a circle.
For the calculations, the curvature of bent windows has been approximated to be that of an arc of a circle. Figure 12 shows the optical path of a ray with angle $\alpha$ and corresponding change of focal point. For this geometry, changes in focal distance ($df$) and optical path difference (OPD) between bent and flat windows have been found. Because of the stiffness of sapphire, we are able to use a much thinner sapphire window. Figure 13 shows change of focal distance ($df$) versus focal length ($f$) for normal incidence for both sapphire and fused quartz. For sapphire, $t=0.2$ mm and for fused quartz, $t=0.6$ has been used. Also, we have assumed that the objective is in contact with the window. Therefore, focal distance is roughly the distance between the atom and the farther surface of the window. The window is a 15 mm X 15 mm square. According to this figure, displacement of focal point due to bending increases with focal distance. For objectives with N.A. $>0.9$ which their focal distance is about 0.3 mm, $df \ll \lambda$, and therefore the effect of bending is negligible. Due to the possibility of rupture, we can only use sapphire windows with these objectives. For objectives with smaller numerical aperture, the higher working distance allows us to use fused quartz. In this case, the change of focal distance is considerable and needs more care. However with these objectives, change of working distance and therefore, aberration is more for sapphire. So we only consider fused quartz in this case. Hereon, we assume that $f=0.3$ mm for sapphire and $f=2$ mm for fused quartz.

Figure 13  Change of focal distance for normal incident
Figure 14 shows dependence of deviation of optical path difference ($\Delta W$) on incidence angle for different thicknesses. $L = 1.5$ cm for both sapphire and fused quartz windows. At the top corner, standard deviations of OPDs are given (at $\lambda = 405\, \text{nm}$). Fused quartz with $t>0.5$ mm and sapphire with at least $t>0.150$ mm are acceptable windows. For sapphire, equation (44) is not valid for $t<0.15$ mm, thus in the figure $t<0.15$ is not shown.

![Figure 14](image)

### 3.5. Birefringence in sapphire

Sapphire is a uniaxial crystal. Its ordinary and extraordinary axes have different indices of refraction. In order to decrease the birefringence effect, we need to use the c-axis window in which ordinary axis is perpendicular to the surface. However, in high numerical aperture objectives where the collection angle is big, using only the c-axis window cannot guarantee birefringence-free performance. In this case, the incident ray can decompose into ordinary and extraordinary rays and with different refraction angles. Therefore, this effect will induce extra optical path difference between ordinary and extraordinary rays which is proportional to the thickness of the window. In addition, the converging point of the ordinary and extraordinary rays arriving at the objective, will be different and also angle dependent. This effect will determine the maximum possible thickness of the sapphire window.
Refraction angle of ordinary and extraordinary rays in uniaxial crystal windows satisfy the following Snell laws

\[
\sin \theta = n_o \sin \theta_o, \\
\sin \theta = n(\theta) \sin \theta_e.
\]  \hspace{1cm} (45)

\(\theta\) is the angle between the electromagnetic wave vector and the ordinary optical axis of the crystal. \(n_o\) and \(n_e\) are ordinary and extraordinary indices of refraction and \(n(\theta)\) is given by [29]

\[
n(\theta) = \frac{n_o n_e}{\sqrt{n_o^2 \sin^2 \theta + n_e^2 \cos^2 \theta}}. 
\]  \hspace{1cm} (46)

Using simple ray optics, the optical path difference and the difference in focal length between ordinary and extraordinary rays can be found as below

\[
OPD = t\left(\frac{1}{\cos \theta_o} - \frac{1}{\cos \theta_e}\right),
\]

\[
df = f_o - f_e = \frac{t}{\tan \theta} (\tan \theta_e - \tan \theta_o). \hspace{1cm} (47)
\]

The amplitude of \(df\) is an increasing function of \(\theta\). Figure 15 shows the relation between \(df\) and thickness for \(\theta = 0.4\pi\). Here again, we have used \(\lambda = 405\) nm. According to this figure, if we have \(df < \lambda / 2\), thickness must be kept less than 0.2 mm.

![Figure 15](image)

Figure 15  change of focal point versus thickness for \(\theta = 0.4\pi\)
Figure 15 shows the optical path difference between ordinary and extraordinary rays for \( \theta \leq 0.4\pi \) or equivalently for a lens with N.A.=0.95. Values of the standard deviation of OPDs are given at the top of the figure. The extraordinary part of the beam does not satisfy the Marechal criterion at all. At \( \theta = 0.4\pi \), the intensity of the transmitted extraordinary beam is roughly 80% of the total intensity, which is a considerable amount. For N.A.=0.75 and \( t=0.15 \text{ mm} \), \( \sigma/(\lambda/14) \approx 1. \) In order to be diffraction limited for both ordinary and extraordinary rays, the numerical aperture must be less than 0.75.

![Figure 16](image)

**Figure 16  Dependence of OPD on angle of incident.**

### 3.6. Effect of index of refraction

Objectives are already aberration corrected for fused quartz coverslips. The difference between indices of refraction of sapphire and fused quartz, will cause further changes in the dependence of focal length on the angle. The purpose of this section is to find the answer the question - is a sapphire window equivalent to a thicker quartz window? And what is that thickness? Displacement of focal length due to an optical window can be written as

\[
\Delta f = f - f_{\text{window}} = t - \frac{t \cos(\theta)}{(n^2 - \sin^2(\theta))^{0.5}},
\]

where \( f \) is the focal length of the lens without coverslip and \( f_{\text{window}} \) is the focal length with coverslip which is generally dependent on the angle. Objectives that have been designed
to work with coverslip, have been corrected for this displacement due to fused quartz coverslips. For the rest, we will define
\[
df_0 = \Delta f_{\text{sapphire}}(t_s)\big|_{\theta=0} - \Delta f_{\text{quartz}}(t_q)\big|_{\theta=0},
\]
where \( t_s \) is the thickness of sapphire and \( t_q \) is the thickness of quartz window. \( df_0 \) is the change of focal length very close to normal incidence.

For the case when the objective is in contact with the window, to have \( df_0 = 0 \), we should have a sapphire window with thickness \( t_s \) less than that of the specific fused quartz window. By equating \( \Delta f_{\text{quartz}} \) and \( \Delta f_{\text{sapphire}} \) from (48), the corresponding thickness can be found to be
\[
t_q = t_s \frac{(n_s-1)n_q}{(n_q-1)n_s} \approx 1.38 t_s.
\]

Figure 17 (a) shows this situation, where after changing the windows, the atom is still at the focal point of the lens.

![Figure 17](image-url)
has been pushed back and simultaneously, the thickness of the sapphire window has been adjusted to keep the atom at the focal point. The thickness of the equivalent quartz window has been found by maximizing Strehl ration.

Figure 18 shows $df$ versus angle for different thicknesses of sapphire. $t_q$ is obtained from (50). For all the shown thicknesses, $\sigma$ is of the order of 100. Although with these thicknesses, the focal lengths of both windows are the same, the induced aberration due to sapphire window is huge.

![Figure 18](image)

Figure 18  Induced change of focal length versus angle when a sapphire window is replaced by its equivalent fused quartz window from (50).

In order to minimize $\sigma$, we adjusted two parameters - $t_q$ and the distance between the objective lens and the sapphire window. Figure 19 shows the dependence of $\sigma$ on the thickness of the quartz window for different thicknesses of sapphire. Distance between the objective and the sapphire window have been adjusted so as to keep the atom at the focal point of the lens. According to this figure, the corresponding thickness of quartz window for minimum aberration is only a few $\mu m$ more than the thickness of the sapphire window. $\sigma$ decreases slowly with decreasing $t_s$ but is still big for $t_s=0.125$ mm. For this thickness, $\sigma = 3.6(\lambda/14)$, where $\lambda = 405$ nm.
Figure 19 Dependence of $\sigma$ on thickness of quartz window. We have assumed that the objective has been aberration corrected for the thickness of quartz window. Substitution of quartz with sapphire, even when the atom is kept at the focal point, induces aberration. The minima in these curves show the points of minimum induced aberration.

In order to further decrease $\sigma$, for sapphire, we displace the objective further backward, but in this case atom is not at the focal point anymore. Figure 20 shows this situation for $t_s=0.15$ mm. With a displacement of only 1.25 $\mu m$, the optics reaches the diffraction limited condition $\sigma\approx0.3(\lambda/14)$. However, as a result of the atom being off-focus, we must work with a slightly convergent beam for imaging. Sortais et al. in their experiments have experienced a similar effect [14]. They imaged a single atom in a tight optical trap with a N.A.=0.5 lens placed inside the vacuum. They noticed that after removing the coverslip, by using slightly out-of-focus imaging, it is possible to reach the diffraction limited condition.

These calculations were for the total collection angle of $\pi/2$ or equivalently N.A.=0.7. For N.A.=0.9, for the best case, $\sigma=1.9(\lambda/14)$ is reached for a displacement of 1.54 $\mu m$. So, for high numerical aperture, optics cannot be diffraction limited.
3.7. Summary

In this chapter, we evaluated different sources of aberration in optical windows. We showed that for N.A.>0.9, due to rupture, using a sapphire window is a must. But because of birefringence of a sapphire crystal and the difference of its index of refraction from that of the standard coverslip, the optics cannot remain diffraction limited.

Fused quartz is a standard coverslip; therefore objectives are already aberration corrected for typical effects. However, a thin layer of fused quartz can not withstand atmospheric pressure and therefore, cannot be used for high numerical aperture objectives, due to their small working distance. According to sections 3.3 and 3.4, the minimum possible thickness of fused quartz for a 15 mm x 15 mm optical window, is about 0.5 mm.

For the case of sapphire windows, in section 3.6, we showed that for N.A.<0.75, by going slightly off-focus, the diffraction limited situation can be recovered. Therefore, sapphire like fused quartz can be used for N.A.<0.75 objectives.
4. Microscope objectives

Because of extensive applications of microscopy in biological research, optical companies have put large efforts into producing high quality objectives and introducing novel microscopy techniques. Today, in addition to biological applications, these highly engineered objectives have found their way into industry. Microscope objectives have a long history, began in 1880’s when Ernest Abbe, Carl Zeiss and Otto Schott developed their achromatic objectives.

Corresponding to the extent of aberration correction and flatness of the field; there are different classes of objectives. Achromatic objectives are the lowest quality level and plan apochromat objectives are the most highly corrected objectives.

The Focal plane is perpendicular to the optical axis at the focal point of the lens. Field curvature is an optical artifact corresponds to the curvature of the image surface (Petzval surface) of the focal plane. Objectives with a flat Petzval surface can be identified by the prefix Plan. Table 5 shows the typical classes of objectives and the wavelengths in which they are corrected for at least one kind of aberration [30].

<table>
<thead>
<tr>
<th>Objective class</th>
<th>Correction Wavelength (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Achromat</td>
<td>486, 546,656</td>
</tr>
<tr>
<td>Plan achromat</td>
<td>436, 486, 546,656</td>
</tr>
<tr>
<td>Fluorite</td>
<td>436, 486, 546,588,656</td>
</tr>
<tr>
<td>Plan fluorite</td>
<td>436, 486, 546,588,656</td>
</tr>
<tr>
<td>Plan apochromat</td>
<td>405, 436, 486, 546,588,656</td>
</tr>
</tbody>
</table>

For determining of the quality of the correction of aberration, the Strehl standard is usually used. According to this standard, the Strehl ratio (S) greater than 0.95 corresponds to excellently corrected, 0.92<S<0.95 to very well, 0.88< S=0.92 to well and
0.82 < S < 0.88 to almost aberration corrected [31]. Fluorite objectives are well diffraction limited at 767 nm, but they are not diffraction limited at 405 nm. Apochromat objectives are almost diffraction limited at 405 nm and well diffraction limited at 767 nm [32].

Microscope objectives have been customized according to their usages in different microscopy techniques. Objectives which are designed for phase contrast microscopy, have an extra diaphragm placed inside. Therefore, we are only interested in non-phase contrast objectives. Dark field and bright field microscopies are the counterparts of fluorescence and absorption imaging.

Most biological applications of microscopy utilize a cover glass to protect specimens. As we discussed in the previous chapter, a coverslip especially in high numerical aperture objectives, introduces spherical aberration. For this reason, some objectives are aberration corrected for the induced aberration due to standard coverslips. The variation of coverslip thickness will significantly increase the aberration in high numerical aperture objectives. Also in some non-biological applications, coverslips with greater thicknesses are needed. Therefore in high numerical aperture objective series, some objectives are designed with correction collars. The correction collar is a ring, which by changing the relative distances of lens components inside the objective, can compensate for different thicknesses of the coverslip. For objectives with N.A. = 0.6, thickness differences (dt) of about 2 mm can be corrected. On increasing the N.A., the range of possible cover glass thicknesses and working distances of the objective dramatically decrease. All apochromat objectives with collar correction have N.A. > 0.9. In microscopy, the cover slip is always in contact with the specimen, and the working distance is defined as the distance between the front lens of the objective and the closer surface of the coverslip. In our application, the definition of working distance changes but yet the sum of the working distance and the coverslip thickness is the distance between the front lens of the objective and atoms. Table 6 shows the typical values of working distances and thicknesses of coverslips for different N.A for objectives with correction collar.
Figure 21 shows the difference between today’s infinity-corrected and older non-infinity-corrected objectives. In older objectives, the image is produced at a fixed distance from the objective (tube length). Adding optical accessories like beam splitters and dichroic mirrors between the image plane and the objective will increase the optical path and introduce spherical aberration. Also, passing converging light through inclined glasses causes ghost images. For these reasons, major microscope manufacturers introduced the standard of infinity-corrected objectives in the 1980s. The image plane of an infinity-corrected objective is located at infinity, therefore to obtain the image, we need to use a tube lens which can be a simple achromatic doublet. Leica, Zeiss, Nikon and Olympus are the highest ranked manufacturers of research and industry grade objectives. Different magnifications at different wavelengths will introduce lateral chromatic aberration in the

**Table 6  Typical characteristics of objective lenses with correction collar**

<table>
<thead>
<tr>
<th>N.A.</th>
<th>W.D. (mm)</th>
<th>Thickness (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.6</td>
<td>2.5-3.5</td>
<td>0-2</td>
</tr>
<tr>
<td>0.75</td>
<td>1.5-2.2</td>
<td>0.5-1.5</td>
</tr>
<tr>
<td>0.9</td>
<td>0.2</td>
<td>0.11-0.23</td>
</tr>
</tbody>
</table>

**Figure 21  Infinity-corrected (left) and non-infinity corrected objectives (right)**
image. Leica and Zeiss correct lateral chromatic aberration with tube lens [30]. Nikon and Olympus apply all the corrections in the objectives. However, because we are imaging only at one wavelength, lateral aberration is not an issue and we are able to use a simple achromatic doublet lens in all cases.

Magnification of infinity corrected objectives is given by the ratio of the focal length of the tube lens (reference focal length) to the focal length of the objective. Therefore, the focal length of the tube lens must be chosen according to the magnification and focal length of the objective. Larger focal lengths will increase the magnification. Table 7 shows the standard reference focal lengths and parfocal distances of Leica, Zeiss, Nikon and Olympus objectives.

<table>
<thead>
<tr>
<th>Manufacturer</th>
<th>Reference focal length (mm)</th>
<th>Parfocal distance (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Leica</td>
<td>200</td>
<td>45</td>
</tr>
<tr>
<td>Zeiss</td>
<td>165</td>
<td>45</td>
</tr>
<tr>
<td>Nikon</td>
<td>200</td>
<td>60</td>
</tr>
<tr>
<td>Olympus</td>
<td>180</td>
<td>45</td>
</tr>
</tbody>
</table>

The distance between objective and tube lens is called infinity space and is typically 11-13 cm. Larger distance will reduce the collection efficiency of the tube lens and decrease the total photon number reaching the detector.

### 4.1. CTF and MTF function

So as to resolve small details of an image in the presence of noise, we need enough contrast. Contrast of a periodic pattern is the ratio of the difference between maximum and minimum to their sum. Standard periodic patterns for derivation of the contrast are sine waves and bar patterns. The dependence of the contrast on frequency for sine waves is called modulation transfer function (MTF). For bar patterns, which we usually use in the lab as test objects, this is called contrast transfer function (CTF). In fact, MTF function is the frequency response of the optics. When the optical system is linear, CTF...
function can be derived from MTF, simply by Fourier expansion of the bar pattern. Also expansion of MTF in terms of CTF is given in [33]

\[
MTF(f) = \frac{\pi}{4} \left[ CTF(f) + CTF(3f) / 3 - CTF(5f) / 5 + ... \right].
\] (51)

In the limit of high frequencies, we can neglect higher order terms

\[
MTF(f) \sim \frac{\pi}{4} CTF(f).
\] (52)

In the low frequency limit, both CTF and MTF are equal to one. Here for the bar patterns, it is assumed that the widths of the dark and bright bars are the same and equal to one half of the period. When the widths are not the same, like in CDs and DVDs, the relation between MTF and CTF is different.

### 4.2. Change of contrast by nonstandard coverslips

In our experiment, absorption and fluorescence imaging at 767 nm are possible by Fluorite objectives, when considering the extent of aberration correction and availability of sufficient working distance. For 405 nm imaging and confocal imaging, we must use the apochromat objectives to have diffraction corrected optics. However, the low working distances of these objectives (0.11-0.23 mm) will greatly restrict optical access of lattice beams. In addition, a 0.17 mm fused quartz window can not be used as the vacuum window. High numerical aperture objectives without correction collar can offer 2-4 times higher working distances, but in the presence of non-standard coverslips when the atom is not at the focal point, they do not preserve diffraction limited performance.

Also, in order to evaluate the performance of an objective, we need to know its MTF function at our required wavelengths. However, these data, if at all, are private and the manufacturers do not give them out.

In order to find the resolution of apochromat and fluorite objectives at our wavelengths and derive their MTF function, we performed some tests on them. Maximum available optical target frequency to our knowledge was 645 lines per mm, which is not sufficient
for us [34]. Therefore, we have used a DVD as our target. The track pitch of DVDs is 740 nm and their width is about 250 nm. For measuring the MTF, a 100% contrast target or a target with a continuum of the frequencies from low frequencies to high frequencies is needed. DVD does not fulfill this requirement. However it can be used to measure the reduction of contrast due to coverslips.

As mentioned earlier, we are not able to use diffraction limited objectives at 405 nm. However, as stated in section 3.6, by going slightly off-focus, it is possible to improve the aberration. Here we are interested in checking this improvement. Table 8 shows the measured contrast of the images of DVD tracks in the presence of various coverslips. We have used a plan fluorite objective with N.A.=0.8 and 100× magnification. By a #181 Lee filter, the green and red part of the spectrum was filtered. The center of the spectrum is roughly 430 nm and its width is about 100 nm. The light power and illumination time in all cases are the same. The last column shows the over estimated Strehl ratio of the optical system in the presence of the coverslip. We discuss the assumptions of this measurement below.

![Table 8](image)

<table>
<thead>
<tr>
<th>Cover slip</th>
<th>Count max</th>
<th>Count min</th>
<th>Contrast%</th>
<th>Uncertainty</th>
<th>Strehl ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Without cover slip</td>
<td>111</td>
<td>10</td>
<td>83</td>
<td>4</td>
<td>~1</td>
</tr>
<tr>
<td>Quartz 0.2 mm</td>
<td>72</td>
<td>13</td>
<td>72</td>
<td>7</td>
<td>&lt;0.64</td>
</tr>
<tr>
<td>Quartz 0.75 mm</td>
<td>52</td>
<td>25</td>
<td>35</td>
<td>3</td>
<td>&lt;0.46</td>
</tr>
<tr>
<td>Sapphire 0.125 mm</td>
<td>69</td>
<td>15</td>
<td>64</td>
<td>4</td>
<td>&lt;0.62</td>
</tr>
</tbody>
</table>

Figure 22 shows the contrast function of a diffraction limited objective lens for a periodic point source object. The numerical aperture of the lens is 0.8 and the wavelength of the light is 430 nm. Diffraction pattern of each point source is an Airy pattern and the contrast is calculated by the addition of Airy patterns.
Figure 22  Contrast of a diffraction limited objective lens versus frequency. Here N.A.=0.8 and $\lambda=430$ nm. The contrast is calculated for the image of periodic point sources. The vertical line shows the repetition frequency of the tracks for DVD.

From Table 5, it is reasonable to assume that the tested objective is diffraction limited at 430 nm. This means that the expected contrast of the DVD image is close to 100% and therefore, from Table 8, the resultant 83% of contrast in the image is due to the contrast of DVD itself. By this assumption, we can estimate the Strehl ratio of the optics in the presence of the coverslips as the ratio of the maximum count number to the maximum count number without coverslip. According to Table 8, “Olymous LMPlanFl 100x/0.80”, in the presence of these coverslips, even at the best off-focus point, is not diffraction limited at 430 nm. However, for the separation of 740 nm, in all cases, the tracks could be resolved. The reduction of the contrast (or MTF) for this separation due to coverslips can be estimated as the ratio of the stated contrast to contrast without coverslip.

4.3. Summary

For imaging at 767 nm, diffraction-limited objectives with high working distance and with correction collars are available. For imaging at 405 nm, objectives with correction collars are not diffraction limited or do not have sufficient working distance. There are
two possible solutions. Firstly, we can work with larger separations and higher intensity of lattice beams and in the non-diffraction limited condition. Secondly, we can use apochromat objectives without correction collar, but designed for standard coverslips. In this case, if we work off-focus, we might be able to recover diffraction limited condition. One of the best objectives for this purpose is “Nikon CFI Plan Flour 20x/0.75”. This objective has a working distance of 1 mm.

In section 2.6, for calculation of needed photon number, we have assumed the diffraction limited situation. For the first approach where the optics is not diffraction limited, we need an optical target to determine the MTF of the objective and then with these new MTF, determine the separation and lattice intensity for which we can achieve the required percentage of correct detection.

For the second approach, we need to make our microscope with 405 nm laser source and measure Strehl ratio with sapphire coverslip. For the measurement of Strehl ratio, we need a high contrast target with sub-resel (< 330 nm) detail. A DVD is a good target for this purpose but for a trustworthy measurement, the real contrast of the DVD itself must be determined.
5. Conclusions

In chapter two, we have shown the possibility of absorption imaging at 767 nm and confocal imaging with the 405 nm excitation. In chapter three, it is shown that due to aberration, objectives with N.A. greater than 0.75 can not be used. Finally in chapter four, we discussed possible microscope objective lenses that can be used for imaging at 405 and 767 nm. Objectives with collar correction and N.A. < 0.75 are not diffraction limited at 405 nm.

For the future, we have two possibilities. First, we can decide to image at 767 nm. In this case, we could use a semi-apochromat objective with correction collar and with N.A. ≈ 0.7. Vacuum window should be a 0.5-0.6 mm thick fused quartz slab. The best S/N is achieved for lattice spacing of about 1 µm (Figure 10). However, imaging even with a lattice spacing around 0.9 µm, is possible; but the required number of scatterings per atom increases about 3 times. Lattice spacing of about 0.95 µm is a good compromise between high S/N and small lattice spacing.

Confocal imaging is the second possibility. In this case we can use two approaches. In the first one we use a long working distance apochromat objective with a fixed coverslip thickness (without correction collar). Then, different sapphire windows a bit thicker than standard coverslip(1-5 µm) must be tested in the off-focus scheme to achieve the diffraction limited condition (Figure 19 and Figure 20). In case of success, lattice spacing of about 0.6-0.7 µm is achievable.

In the second approach, a semi-apochromat objective with collar correction can be used. Because the objective is not aberration corrected, the point spread function is broader. In order to keep the contrast unchanged, lattice spacing must be increased. We estimate that this increase is less than 25%. Therefore, in this approach, a lattice spacing greater than 750 nm is acceptable. The actual width of the point spread function must be tested.
References:


[34] For example high resolution 1951 USAF Target by Edmond optics.