Spatial resolution below the diffraction limit in air has been achieved with solid immersion microscopy, in which light focused through a solid immersion lens (SIL) forms a spot at the bottom surface of the lens. A sample held in the near field of the focused spot can be imaged with spatial resolution limited by diffraction in the solid. With a hemispherical SIL, spatial resolution is smaller than that in air by a factor equal to the refractive index of the lens, according to the vector diffraction theory of Richards and Wolf, which completely specifies the electric and magnetic field vectors at a focus many wavelengths away. SIL’s larger than 1 mm in diameter have been used for imaging, data storage, and photolithography. Recently a Si SIL with a diameter of 15 μm and demonstrated λ/5 resolution at a wavelength of λ = 9.3 μm was microfabricated. However, vector diffraction theory cannot be used to predict focused spot size in lenses this small.

When lens diameter is reduced to nearly the wavelength of light, diffraction of the input beam at the lens surface causes variations in phase and amplitude that affect focusing inside the lens. An extreme example of the breakdown of diffraction theory occurs for the electrostatic case when the lens diameter is much smaller than the wavelength and the fields become uniform across the lens. For lens diameters of the order of the wavelength, scalar diffraction theory and the vector diffraction theory of Richards and Wolf cannot be used to predict the spatial distribution of field amplitudes.

In this Letter we examine the fields within a spherical Si microlens illuminated by a converging wave and investigate the effects of the lens’s radius of curvature, maximum illumination angle, and refractive index on fields near the focus. Our results show that vector diffraction theory overpredicts the spot size in Si microlenses smaller than 4λ in diameter. Changes in maximum illumination angle have little effect on the focus in Si microlenses smaller than a wavelength in diameter, and changes in index do not cause the proportional changes in spot size that would be expected from vector diffraction theory.

We consider the case of a Si sphere (n = 3.4) with diameter d illuminated by a converging wave with wavelength λ and maximum illumination angle θ, as shown in Fig. 1, in which the illumination numerical aperture (NA) is sin θ in air. The illuminating wave propagates in the positive z direction and is focused by an objective to the center of a Si sphere suspended in air. Fields within a sphere illuminated by a plane wave can be calculated according to Mie theory, for which the standard derivation can be found in many references. Fields within a sphere illuminated by a converging wave are obtained here by use of an extension of Mie theory.

We start by defining two vectors, \( \mathbf{M} = \nabla \times (c \psi) \) and \( \mathbf{N} = (\nabla \times \mathbf{M})/k \), where \( \psi \) is a scalar function that satisfies the scalar wave equation, \( k \) is the wave number, and \( c \) is an arbitrary constant vector. It can be shown that \( \mathbf{M} \) and \( \mathbf{N} \) have all the required properties of an electromagnetic field. The fields in the incident converging wave are given by Richards and Wolf in terms of integrals over the maximum illumination angle. The incident converging wave \( \mathbf{E}_0 \) can be expanded in vector spherical harmonics according to

\[
\mathbf{E}_0 = \sum_{m=0}^{\infty} \sum_{n=m}^{\infty} (A_{mn} \mathbf{M}_{mn} + B_{mn} \mathbf{N}_{mn}),
\]

Fig. 1. Schematic of a spherical microlens of diameter \( d \) and index \( n \) illuminated by a converging wave of wavelength \( \lambda \) at a maximum angle \( \theta \).
where the coefficient $A_{mn}$ is given by

\[
A_{mn} = \frac{\int_0^{2\pi} \int_0^{\pi} \mathbf{E}_0 \cdot \mathbf{M}_{mn} \sin \theta d\theta d\phi}{\int_0^{2\pi} \int_0^{\pi} |\mathbf{M}_{mn}|^2 \sin \theta d\theta d\phi}
\]

and $B_{mn}$ is given by a similar expression. Like the incident wave, the internal and scattered fields, $\mathbf{E}_i$ and $\mathbf{E}_s$, respectively, can be written in terms of the vector spherical harmonics $\mathbf{M}$ and $\mathbf{N}$. The incident waves ($\mathbf{E}_0$ and $\mathbf{H}_0$), external scattered fields ($\mathbf{E}_e$ and $\mathbf{H}_e$), and internal fields ($\mathbf{E}_i$ and $\mathbf{H}_i$) are related at the sphere’s surface by the boundary conditions $(\mathbf{E}_0 + \mathbf{E}_e - \mathbf{E}_i) \times \mathbf{e}_{r=0} = 0$ and $(\mathbf{H}_0 + \mathbf{H}_e - \mathbf{H}_i) \times \mathbf{e}_{r=0} = 0$. These conditions require that the tangential components of the external and internal field be continuous at the interface.

Since the expression for the incident electric field requires integration over the maximum illumination angle, it is not possible to find a general analytical expression for the internal and external fields. Instead, the equations are numerically integrated to yield expansion coefficients for the incident converging wave. The internal fields are reconstructed from expansion coefficients obtained through the boundary condition relations, and the results are presented in terms of the Poynting vector, $\mathbf{S} = \frac{1}{2} \text{Re} \{\mathbf{E}_i \times \mathbf{H}_i^*\}$, in the direction of propagation ($S_z$) as a function of radial distance normalized by wavelength. Although the SIL is normally close to a hemisphere in shape, we use a full sphere in the model for simplicity. The effect of a plane exit face on the focused beam shape is expected to be small based on comparisons with a modified vector diffraction theory that accounts for reflections at the exit face.10 The primary resonance peaks predicted for a sphere from Mie theory exist for dimensions smaller than those considered here, although higher-order resonances may affect field amplitudes within the sphere.14

Figure 2 shows the radial distribution of $S_z$ within spheres of diameter $4\lambda$, $2\lambda$, and $\lambda$ for an illumination NA of 0.8. The fields are plotted at the position along the $z$ axis of maximum $S_z$ for $\phi = \pi/2$, where $\phi$ is an angle relative to the initial polarization of the incident wave. As the sphere diameter is reduced, the FWHM of the focused spot is reduced to 0.18$\lambda$, 0.16$\lambda$, and 0.14$\lambda$, respectively, and the position along the $z$ axis of maximum $S_z$ approaches the location predicted for an incident plane wave. For these lenses, the calculated spot sizes are more than 5% and up to 25% smaller than the FWHM of 0.19$\lambda$ expected from vector diffraction theory for a sphere. The spot sizes for other values of $\phi$ vary by approximately 1% from the mean. Lenses smaller than approximately $\lambda/3$ in diameter no longer focus light to a central spot and approach a uniform field distribution across the sphere with further reduction in diameter.

The size of a focused spot is inversely proportional to the illumination NA, according to vector diffraction theory. For spheres that are close to the wavelength in diameter, calculations show that NA has a diminishing effect on the focused spot size as sphere diameter decreases. Figure 3 gives the radial distribution of $S_z$ within a sphere of diameter $\lambda$ for illumination NAs of 0.8, 0.6, 0.4, and 0.2 at $\phi = \pi/2$. The differences in the FWHM of the spots are less than 2% from 0.14$\lambda$. The focused spot created by the incident converging wave is nearly the same size as that created by an incident plane wave, as shown by the Mie theory results plotted for comparison in Fig. 3.

Reducing the index of refraction of the sphere increases the effective wavelength inside the lens without changing the excitation fields on the lens surface. Figure 4 shows the radial distribution of $S_z$ within a sphere of diameter $2\lambda$ for $n = 3.4$ and $n = 1.7$ with an illumination NA of 0.8 at $\phi = \pi/2$. The spots predicted by vector diffraction theory for an infinite sphere with $n = 3.4$, 1.7, 1.0 are also shown. Decreasing the index of the refraction by a factor of 2 increases the spot size by a factor of 1.7 instead of the factor of 2.0 expected from vector diffraction theory.

In conclusion, we have shown that diffraction at the surface of a microlens illuminated with a converging wave becomes significant as the diameter approaches the wavelength. For Si lenses with diameters smaller than $4\lambda$, focused spots are predicted to be as much as

![Figure 2](image337x311to536x466)

**Fig. 2.** Variation in spot size with Si microlens diameter for $d = 4\lambda$, $2\lambda$, $\lambda$ for a NA of 0.8 at $\phi = \pi/2$. The dotted curve shows the spot expected from vector diffraction theory.1

![Figure 3](image338x87to536x242)

**Fig. 3.** Variation in spot size with illumination NAs of 0.8, 0.6, 0.4, and 0.2 in a Si microlens of diameter $\lambda$ at $\phi = \pi/2$. The dotted curve shows the spot expected from Mie theory.
Fig. 4. Variation in spot size with index of refraction $n = 3.4, 1.7$ in a Si microlens of diameter $2\lambda$ for a NA of 0.8 at $\phi = \pi/2$. The solid curves show results from the converging wave model, and the dashed curves show the spots expected from vector diffraction theory.

25% smaller than those given by vector diffraction theory. Reduction of the index of refraction by a factor of 2 increases the spot size less than would be expected from vector diffraction theory. These properties must be considered in predicting and evaluating the performance of microfabricated lenses that are close to a wavelength in diameter.

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References