

Collecting fluorescence from color centers in bulk materials via the near field of a nanofiber

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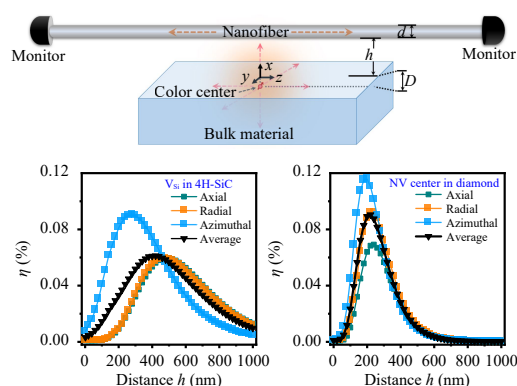
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ABSTRACT

Rapid detection and precise characterization of color centers in semiconductor materials have become pivotal challenges in advancing color-center-based quantum technologies. Here, we propose a non-invasive near-field detection scheme that employs a silica nanofiber as a one-dimensional waveguide for fluorescence collection and rapid detection of color centers in bulk materials. Using three-dimensional finite-difference time-domain (FDTD) simulations, we systematically investigate the influence of key parameters on collection efficiency η , including the nanofiber diameter, the distance between the nanofiber and the sample, and the depth of the color center within the bulk material. For two representative color centers, the silicon vacancy in 4H-SiC and the nitrogen-vacancy center in diamond, the optimized peak collection efficiencies are 0.22% and 0.18%, respectively. Unlike previous studies where silica nanofibers were employed for color centers in nanoparticles or free-space emitters, this work extends the application of silica nanofibers to the detection of color centers in high-index bulk materials. The proposed scheme enables one-dimensional line detection that can be extended to two-dimensional planar scanning, allowing rapid, high-throughput and non-invasive characterization. It is inherently compatible with fiber-optic systems and adaptable to various color centers in different host bulk materials. In summary, this work provides a new technical route and comprehensive theoretical parameter guidance for non-invasive, integrable, high-throughput detection of color centers in bulk materials, paving the way for all-fiber integrated quantum photonics.

Keywords color centers in bulk materials, defect detection, nanofiber



1 Introduction

Color centers have emerged as a highly promising physical

platform for quantum technologies and precision measurement applications [1–4]. There exists a wide variety of color centers, including not only the extensively



studied nitrogen–vacancy (NV) center in diamond [2], but also silicon vacancy (SiV) and germanium vacancy (GeV) in diamond [5], silicon monovacancy (V_{Si}) and divacancy (DV) [6] in silicon carbide (SiC), T-center in silicon (Si) [7], and boron vacancy (VB) in boron nitride (BN) [8], among others. Due to their exceptional luminescence properties, high optical stability, outstanding coherence properties, and compatibility with mature processing techniques, these color centers are widely applied in quantum computing [2, 3], quantum networks [9–11], quantum sensing [12, 13], and quantum imaging [14, 15].

Color centers can generally be fabricated into either bulk materials or nanoparticles, contingent upon the specific applications. For example, in comparison to the NV centers in nanodiamonds, those situated in ultra-pure bulk diamonds exhibit reduced nitrogen impurity concentrations and more stable charge states, thereby enabling significantly longer spin coherence times [16]. Moreover, as opposed to a single-color center, an ensemble of color centers offers higher fluorescence signal intensity. Consequently, ensembles of color centers in bulk materials have increasingly demonstrated distinct advantages across various fields, including super-resolution imaging [15, 17], quantum sensing [12, 18], biomedical detection [14, 19], and so on.

Efficient collection of fluorescence from color centers in bulk materials is crucial for the applications mentioned above. Conventionally, fluorescence from emitters in such bulk materials is collected using confocal microscopy (CM) systems equipped with high numerical aperture (NA) objectives. However, the collection efficiency of an objective is low because it can only collect fluorescence that falls within the solid angle defined by its NA. Even with a high-NA air objective $NA = 0.95$, the limit collection efficiency is only about 3%; while for an oil immersion objective with $NA = 1.49$, the limit collection efficiency remains as low as 10% [20]. Moreover, immersion oil can contaminate the bulk sample during testing, which is often detrimental or even fatal to bulk materials. In addition, the CM systems are generally bulky, costly, and exhibit limited spatial resolution due to the optical diffraction limit [20]. To improve collection efficiency, researchers have developed various micro/nano photonic structures, including solid immersion lenses [21], monolithic immersion metalens [22], microdisk resonators [23, 24], nanopillars [25, 26], and waveguide structures [27]. These structures can enhance directional fluorescence coupling to some extent, but their fluorescence signals still require collection by an objective and thus remain dependent on it. Taking solid immersion lenses as an example, they can increase the collection efficiency to 20%–30% [21]. Nevertheless, these micro/nano photonic structures share common limitations. Their spatial resolution is constrained by their physical dimensions. They require precise alignment with individual

color centers and are therefore unsuitable for high-throughput characterization of color center ensembles. Moreover, their fabrication is complex, costly, and often invasive, easily compromising the integrity of the bulk material. Consequently, for rapid defect detection in integrated devices with complex structures such as quantum chips, a new approach is urgently needed that is non-invasive, easily integrable, low-cost, and capable of directly collecting fluorescence without an objective.

Nanofibers, as powerful tools for fluorescence collection, have attracted significant attention over the past decades [28, 29] due to their advantages such as facile integration, low cost, low optical loss, and the capability to overcome the diffraction limit via subwavelength field confinement. Nanofibers can be fabricated by the flame-brush method, which offers a convenient and economical approach [30]. Nanofibers impose strong transverse constraints on the guided mode due to their subwavelength diameter, resulting in a significant evanescent field on their surface. This strong evanescent field enables nanofibers to serve as an efficient interface for light-atom interaction. The remarkable optical properties of nanofibers have inspired a wide range of applications, including near-field coupling [31, 32], passive optical components [33], optical sensing [34], and fiber lasers to nonlinear optics [35], optomechanics [36], and atom optics [30, 37]. Furthermore, nanofibers have been extended to hybrid quantum experimental systems combined with various quantum emitters, including quantum dots [38, 39], color centers in nanodiamonds [40, 41], single molecules [42], rare earth complexes [43], and two-dimensional materials [44]. Notably, hybrid quantum systems that combine nanofibers with color centers facilitate automatic and alignment-free coupling directly with single-mode fibers [37–44], presenting a promising pathway toward scalable quantum photonic architectures.

In this work, we propose a near-field detection scheme utilizing a nanofiber as a one-dimensional waveguide for efficient fluorescence collection from a color center in a bulk material. A theoretical model is established using the three-dimensional finite-difference time-domain (FDTD) method, and systematic simulations are performed to evaluate the effects of key experimental parameters on the collection efficiency, including the nanofiber diameter, the distance between the nanofiber and the bulk material, and the depth of the color center within the bulk material. Two types of color centers are simulated in this study, namely the V_{Si} in 4H-SiC at its cubic site and NV centers in diamond. As prototypical solid-state quantum emitters in the field of quantum photonics, their distinct material properties and application scenarios enable a comprehensive evaluation of the performance and universality for the near-field coupling scheme of nanofiber and bulk materials. Furthermore, these two types of color centers correspond to mainstream

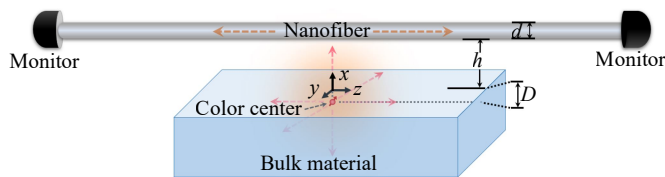


Fig. 1 Schematic of the simulation model. The simulation illustrates the collection of fluorescence from a single color center in a bulk material via a nanofiber. The gray cylinder represents the nanofiber, the blue rectangular prism denotes the bulk material, and the red sphere indicates the single color center. The red sphere schematically indicates the position of the color center within the coordinate system. In the actual modeling, we use the “dipole source” as the color center without considering its shape. Since the emission of the color center is non-directional, fluorescence is simulated for three independent polarization orientations: radial (x -axis), azimuthal (y -axis), and axial (z -axis).

quantum application scenarios in the visible and near-infrared bands, respectively. The conclusions drawn from this study can provide direct guidance for the design of integrated quantum devices operating in different wavebands. Additionally, the effective spatial response of the nanofiber is simulated by varying the transverse distance between the color center and the nanofiber. Previous studies on silica nanofibers have mostly focused on color centers in nanoparticles, free-space emitters, or color centers in pre-fabricated photonic structures. In contrast, this work systematically investigates the near-field fluorescence coupling characteristics of silica nanofibers for deeply embedded color centers in unprocessed bulk materials. Second, we present design rules for key parameters of two representative color centers, offering direct guidance for future experiments. Third, we propose a non-invasive one-dimensional line detection scheme that can be extended to two-dimensional planar scanning, enabling rapid, high-throughput characterization without compromising sample integrity. In summary, the proposed scheme provides an effective technical route for fluorescence collection from bulk color centers and establishes a clear theoretical and parametric foundation for subsequent experiments. Section 2 details the simulation model and methods.

2 Simulation model

Figure 1 schematically illustrates the FDTD simulation model (FDTD Solutions, Lumerical) for collecting fluorescence from a single color center within a bulk material using a nanofiber. In this model, the gray cylinder represents the nanofiber, while the blue rectangular prism denotes the bulk material. The red sphere with an arrow denotes an individual color center within the bulk material. The coordinate system in Fig. 1 has its origin at the

center of the bulk material's top surface. The nanofiber, with a length of $100\text{ }\mu\text{m}$, is positioned so that its center is located at coordinates $(x = h\text{ }\mu\text{m}, y = 0\text{ }\mu\text{m}, z = 0\text{ }\mu\text{m})$, where h represents the distance between the nanofiber surface and the top surface of the bulk material. The diameter of the nanofiber is denoted as d . The material of the nanofiber is SiO_2 with a refractive index of 1.46. The bulk material has dimensions of $6\text{ }\mu\text{m} \times 10\text{ }\mu\text{m} \times 30\text{ }\mu\text{m}$ ($x \times y \times z$), with its center situated at $(x = -3\text{ }\mu\text{m}, y = 0\text{ }\mu\text{m}, z = 0\text{ }\mu\text{m})$. The two types of bulk materials are treated as optically isotropic and dispersion-free throughout the simulations. Diamond is a cubic crystal with an isotropic refractive index of 2.417 at the NV zero-phonon line wavelength of 637 nm. For 4H-SiC, although it is optically anisotropic, the V_{Si} transition dipole moment is confined to the basal plane perpendicular to the c -axis, so the emitted fluorescence is dominated by the ordinary ray. The ordinary refractive index of 4H-SiC is approximately 2.60 at the V_{Si} emission wavelength of 917 nm. Since this work aims to reveal the general physical laws of near-field coupling between a nanofiber and color centers in bulk materials when the crystal orientation is unknown, an isotropic refractive index of 2.60 is adopted for 4H-SiC. Dispersion is neglected because only a single characteristic emission wavelength is simulated for each color center. The color center within the bulk material, located at $(x = -D\text{ }\mu\text{m}, y = 0\text{ }\mu\text{m}, z = 0\text{ }\mu\text{m})$, is modeled using the ‘dipole source’ function in FDTD Solutions, where D denotes the depth below the top surface of the bulk material. The dipole radiates at the zero-phonon line wavelength of the corresponding color center. This single-wavelength setting is consistent with the standard experimental practice of isolating the zero-phonon line via narrowband filtering [45], ensuring that the calculated collection efficiency reflects the actual detectable signal. The present model targets general bulk materials with unknown crystallographic orientation, for which the transition dipoles of color centers are randomly distributed in three-dimensional space. We therefore simulate fluorescence emission for three independent orthogonal dipole orientations: radial (x -axis), azimuthal (y -axis), and axial (z -axis).

It is worth noting that for those color centers in nanoparticles, factors such as particle morphology can significantly affect their coupling efficiency with nanofibers [46]. This more complex scenario is beyond the scope of the present study. Our work focuses on bulk material systems, where treating color centers as a ‘dipole source’ is a well-established and widely accepted approximation for such systems. The computational domain is set to $5.1\text{ }\mu\text{m} \times 2.1\text{ }\mu\text{m} \times 80.1\text{ }\mu\text{m}$ ($x \times y \times z$), positioned with its center at $(x = -1.5\text{ }\mu\text{m}, y = 0\text{ }\mu\text{m}, z = 0\text{ }\mu\text{m})$. All boundaries are set with perfectly matched layers (PML) to eliminate boundary reflections. The simulation employs a nonuniform mesh with minimum step size of 0.25 nm. Mesh convergence tests confirm

that the simulation results are well-converged at this mesh resolution. The time step and simulation time are set to 0.048 fs and 100 ps, respectively. To account for the differing radiation characteristics of optical fields in various directions, the PML layers are configured with 28 layers at the x -boundaries, 28 layers at the y -boundaries, and 16 layers at the z -boundaries, with the PML reflection coefficient set to 1×10^{-9} . Finally, the field monitors are placed at both ends of the nanofiber ($z = \pm 40 \mu\text{m}$) to collect the fluorescence coupled into the nanofiber.

In the simulation model, to quantitatively characterize the fluorescence collection efficiency of our scheme, we perform the following calculations within the FDTD framework. First, to normalize the emission power of the color center, we define two power quantities and a correction factor. $P_0(f)$ is the nominal total radiated power of the dipole source in free space, which is directly output by the FDTD software. $P_{\text{dip}}(f)$ is the actual total radiated power of the identical dipole source when embedded in the bulk material. The power correction factor is defined as $K(f) = P_{\text{dip}}(f)/P_0(f)$, which quantifies the modification of the total dipole radiation power by the high-index bulk material relative to the free-space case. The frequency f corresponds to the characteristic fluorescence emission wavelength of the color center, specifically 917 nm for the V_{Si} in 4H-SiC and 637 nm for the NV center in diamond. The correction factor $K(f)$ accounts for the modification of the dipole radiation by the high-index bulk material, allowing us to correct the collected power from the free-space reference to the actual total radiated power in the bulk. Subsequently, frequency-domain power monitors positioned at both ends of the nanofiber ($z = \pm 40 \mu\text{m}$) cover the full cross-section of the nanofiber and record the total optical power coupled into all guided modes propagating in the $+z$ and $-z$ directions, denoted as T_R and T_L , respectively. The fluorescence collection efficiency η is defined as the ratio of the total guided power coupled into the nanofiber to the total radiation power of the dipole in the bulk material, that is $\eta = (T_R + T_L)/K(f) \times 100\%$. This definition characterizes the intrinsic coupling and collection capability of the nanofiber's evanescent field for fluorescence emitted within the bulk material. It isolates the optical coupling process from alterations to the color center's intrinsic emission rate induced by the surrounding medium, and does not account for coupling losses associated with fluorescence escaping the crystal surface into free space. This formulation provides a rigorous theoretical benchmark for evaluating the performance of corresponding experimental systems.

3 Numerical simulations and discussion

In this section, we conduct a systematic investigation of

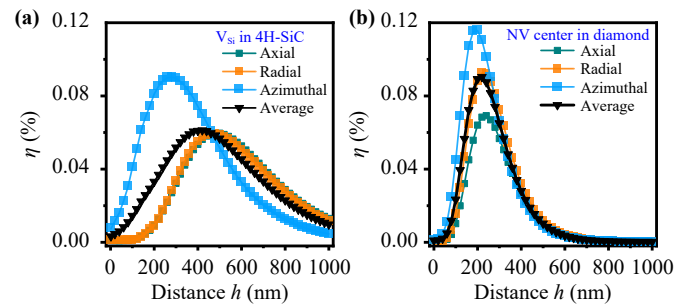


Fig. 2 Simulated fluorescence collection efficiency η for (a) the V_{Si} in 4H-SiC and (b) the NV center in diamond, collected by a nanofiber with $d = 400 \text{ nm}$. The color center is positioned at a fixed depth ($D = 30 \text{ nm}$), and η is plotted as a function of the h for three polarizations: axial (teal solid squares), radial (orange solid squares), azimuthal (blue solid squares). The black solid downward triangles denotes the average collection efficiency over the three polarizations. The optimal h values are 420 nm for the V_{Si} in 4H-SiC and 220 nm for the NV center in diamond.

the proposed scheme through three-dimensional FDTD simulations. First, the feasibility of the proposed scheme is verified. We simulate the collection efficiency η of the fluorescence emitted by two types of color centers in bulk materials, utilizing a nanofiber of diameter $d = 400 \text{ nm}$. The two types of color centers are the V_{Si} in 4H-SiC and the NV center in diamond. The depth D of the color center is set at 30 nm, aligning with the typical implantation depth for generating the V_{Si} in 4H-SiC with 20 keV carbon ions [47].

As shown in Fig. 2, we simulate the variation of η with h when the color center emits fluorescence with the axial, radial, and azimuthal polarizations, respectively. Figures 2(a) and (b) present the results for a nanofiber with a diameter of 400 nm coupled to V_{Si} in 4H-SiC and to NV centers in diamond, respectively. Among these, the collection efficiency η is highest when the color center emits fluorescence with azimuthal polarization. This is because the dipole orientation in this case optimally aligns with the azimuthal electric field component of the fundamental HE_{11} mode of the nanofiber, thereby enabling more efficient coupling into the guided mode [48]. For bulk materials with randomly oriented color center dipoles, we take the arithmetic mean of the collection efficiencies along three orthogonal polarization directions to obtain the final collection efficiency η , which characterizes the overall collection efficiency across all possible dipole orientations. This average collection efficiency η is represented by the black solid downward triangles in Fig. 2. As shown in Fig. 2, a common trend observed for both color centers is that η initially increases and then decreases as h is reduced from 1000 nm to 0 nm, indicating the presence of an optimal h for maximizing η . This phenomenon is attributed to the coupling strength between the evanescent

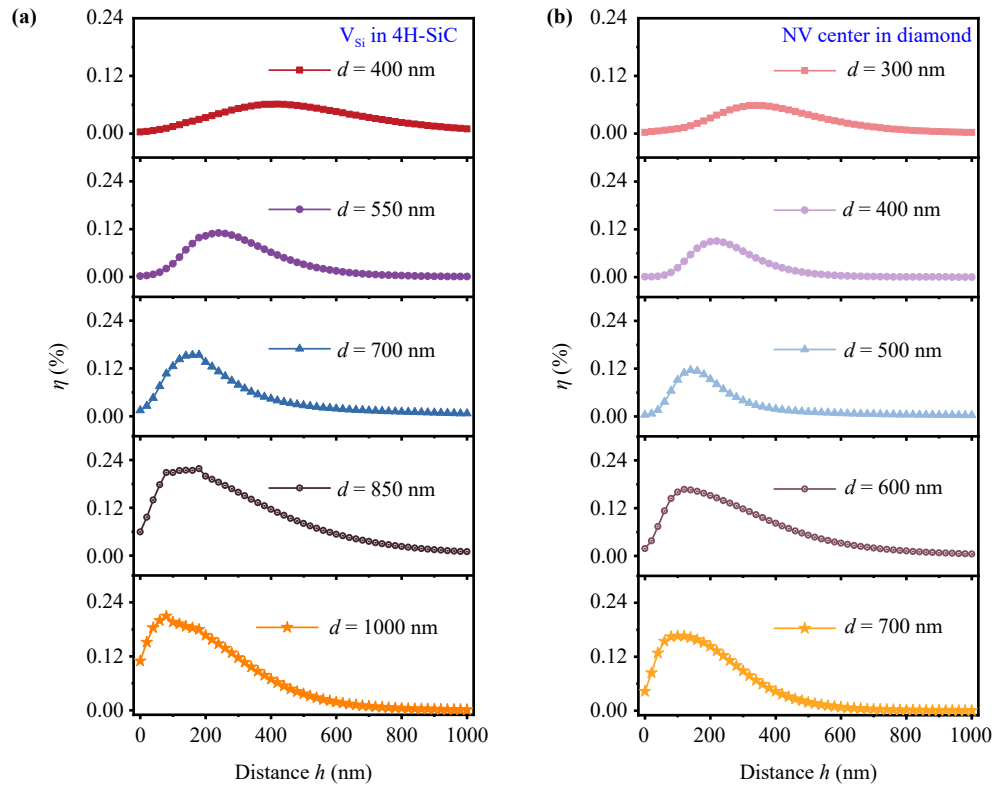


Fig. 3 Simulation results for the V_{Si} in 4H-SiC (a) and the NV center in diamond (b), illustrating the fluorescence collection efficiency η as a function of h for d ranging from 300 nm to 1000 nm. The color centers are fixed at a depth ($D = 30$ nm). Here, only selected data are shown for nanofiber diameters d between 300 nm and 1000 nm.

field on the surface of the nanofiber and the fluorescence of the color center. Specifically, the simulation results reveal distinct optimal values of h for the two types of color centers under identical conditions of d and D . The optimal h is 420 nm for the V_{Si} in 4H-SiC and 220 nm for the NV center in diamond. This discrepancy stems from the decay length of the nanofiber's evanescent field being determined by the fluorescence wavelength of the color center, which is 917 nm for the V_{Si} and 637 nm for the NV center. Furthermore, this is influenced by the high refractive index of the bulk material.

Having verified the feasibility of the proposed experimental scheme, we now systematically investigate the influence of key parameters on the collection efficiency η . To achieve the maximum collection efficiency η , the key geometric parameters d , h , and D are systematically optimized. The evanescent field on a nanofiber surface exhibits exponential decay along the radial direction [49], with the decay range being determined by the nanofiber diameter, the wavelength of guided light and the refractive index of the surrounding medium. Therefore, efficient fluorescence coupling from a color center in a bulk material depends on h and d simultaneously. Initially, we simulate collection efficiency η as a function of distance h for nanofiber diameters from 300 nm to 1000 nm. The results are presented in Figs. 3(a) and (b)

for two types of color centers, V_{Si} in 4H-SiC and NV center in diamond, respectively. From simulation results, we systematically extract the peak values of each curve and their corresponding h . Specifically, the peak value of each curve is defined as the maximum collection efficiency η (η_{max}) for the corresponding d , and the h value at this peak is designated as the optimal distance h (h_{opt}).

To more clearly illustrate the influence of the distance h and the nanofiber diameter d on the collection efficiency η , we present Fig. 4. Figures 4(a) and (b) show the maximum collection efficiency η_{max} and optimal distance h_{opt} as a function of d for the two different color centers. To enhance the physical insight and generality of the results, the upper horizontal axis in each of Figs. 4(a) and (b) denotes the normalized frequency parameter V corresponding to the lower horizontal axis (nanofiber diameter d). The conversion relationship between V and the nanofiber diameter d is given by $V = \frac{\pi d}{\lambda} \sqrt{n_f^2 - n_{cl}^2}$ [48], where λ is the fluorescence wavelength, and $n_f = 1.46$ and $n_{cl} = 1$ are the refractive indices of the nanofiber and the cladding (air), respectively. This representation retains the intuitive diameter scale for experimental convenience while providing a more universal understanding of the waveguide dimension effects.

Figures 4(a) and (b) show the maximum collection efficiency η_{max} and the optimal distance h_{opt} as functions

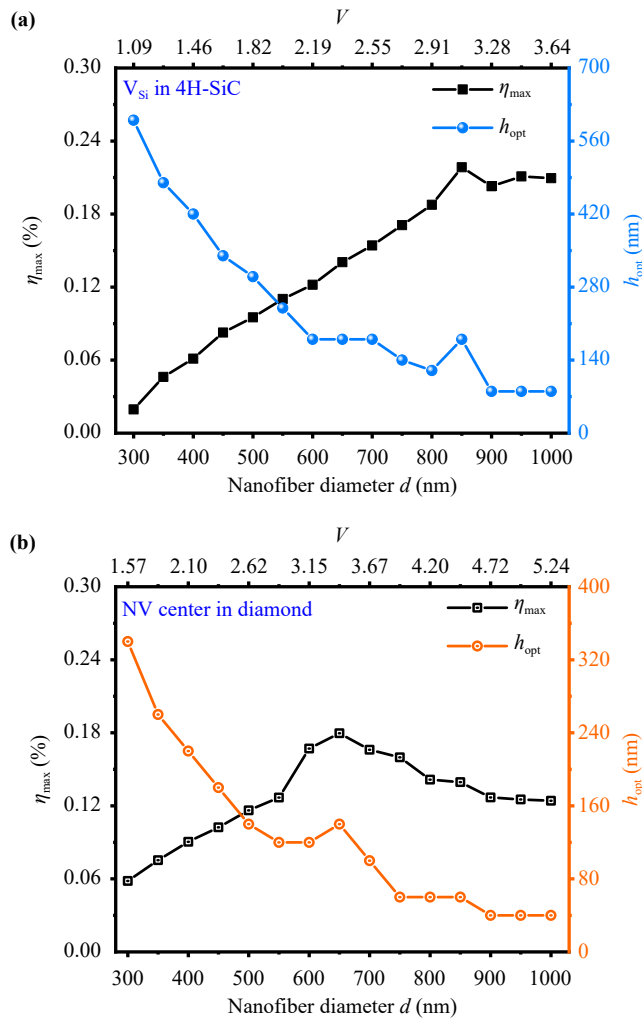


Fig. 4 The maximum collection efficiency $\eta_{\max}$ (left axis) and optimal distance h_{opt} (right axis) as functions of nanofiber diameter d (lower axis) and the normalized frequency parameter V (upper axis), for the V_{Si} in 4H-SiC (a) and the NV center in diamond (b). For the V_{Si} in 4H-SiC, $\eta_{\max} = 0.22\%$ at $d_{\text{opt}} = 850$ nm and $h_{\text{opt}} = 180$ nm; for the NV center in diamond, $\eta_{\max} = 0.18\%$ at $d_{\text{opt}} = 650$ nm and $h_{\text{opt}} = 140$ nm. The conversion is given by $V = (\pi d/\lambda) \sqrt{n_f^2 - n_{\text{cl}}^2}$, with $n_f = 1.46$ and $n_{\text{cl}} = 1$.

of the nanofiber diameter d for the two types of color centers. On the one hand, the coupling behavior of the two types of color centers exhibits consistent trends. First, $\eta_{\max}$ varies nonmonotonically with d for both color centers, reaching a peak at an optimal diameter (d_{opt}). The V_{Si} in 4H-SiC achieves $\eta_{\max} = 0.22\%$ at $d_{\text{opt}} = 850$ nm, while the NV center in diamond reaches $\eta_{\max} = 0.18\%$ at $d_{\text{opt}} = 650$ nm. This nonmonotonic variation of $\eta_{\max}$ with d is attributed to the competition between multimode coupling gain and evanescent field decay in the nanofiber. When the normalized frequency parameter $V < 2.405$, the nanofiber supports only the fundamental HE_{11} mode, and increasing d in this regime enhances the

evanescent field strength, thereby improving collection efficiency. When V exceeds 2.405, the nanofiber transitions to a multimode fiber. At the optimal diameter d_{opt} , where $2.405 < V < 3.832$, the nanofiber operates in the few-mode regime and supports six guided modes for efficient fluorescence transmission. These include two orthogonal polarizations of the fundamental HE_{11} mode and four low-order higher-order modes corresponding to TE_{01} , TM_{01} , and the two polarization degeneracies of HE_{21} , which provide additional multimode coupling gain. Mode decomposition under the optimal parameters reveals that the two orthogonal polarizations of the fundamental HE_{11} mode contribute approximately 60% of the $\eta_{\max}$, with the remaining 40% arising from four higher-order guided modes. Since the tapered nanofiber in experiments collects all guided modes simultaneously and cannot resolve their individual contributions, the $\eta_{\max}$ reported in this work is in direct agreement with experimental measurements. However, further increase of d simultaneously reduces the intensity and radial extension of the evanescent field on the nanofiber surface, weakening the interaction between the nanofiber and the color center [49]. Therefore, d_{opt} is precisely the balance point between multimode coupling gain and evanescent field decay. Moreover, at these specific diameters, an unexpected local resonance enhancement may exist between the fluorescence wavelength and the nanofiber [50]. Second, the optimal distance h_{opt} decreases monotonically with increasing d for both color centers. This is because a larger nanofiber diameter results in a more rapidly decaying evanescent field [49], requiring the nanofiber to be placed closer to the color center to maintain sufficient coupling strength. This trend holds for all simulated diameters.

On the other hand, the optimal parameters d_{opt} and h_{opt} differ quantitatively between the two types of color centers. We attribute this difference to their different emission wavelengths and the refractive indices of the host bulk materials. First, the emission wavelength of the V_{Si} in 4H-SiC is 917 nm, significantly longer than that of the NV center in diamond at 637 nm. Coupling longer-wavelength fluorescence requires a larger nanofiber diameter to reach the same V value and enter the multimode coupling regime [48]. This directly explains why the optimal diameter of the V_{Si} in 4H-SiC $d_{\text{opt}} = 850$ nm is larger than that of the NV center in diamond, $d_{\text{opt}} = 650$ nm. Second, a longer wavelength corresponds to a longer evanescent decay length of the nanofiber [51], allowing the V_{Si} in 4H-SiC to couple efficiently even at larger distances, so its optimal distance $h_{\text{opt}} = 180$ nm is larger than that of the NV center in diamond, $h_{\text{opt}} = 140$ nm. Finally, the high refractive indices of the bulk materials, 2.60 for 4H-SiC and 2.417 for diamond, modify the local density of optical states of the evanescent field and also affect the absolute values of the optimal parameters d_{opt} and h_{opt} . In summary, for

the V_{Si} in 4H-SiC, the optimal parameters are $d_{opt} = 850$ nm and $h_{opt} = 180$ nm; for the NV center in diamond, the optimal parameters are $d_{opt} = 650$ nm and $h_{opt} = 140$ nm. The peak collection efficiencies achieved under these respective optimal parameters are 0.22% and 0.18%. Based on the optimal parameters obtained above, we further analyzed the allowable deviation range of h_{opt} . Taking 90% of the maximum collection efficiency as the performance threshold, the allowable h range for the NV center system is from 76.5 nm to 218.6 nm, and for the V_{Si} system from 72.2 nm to 207.6 nm. Both systems exhibit certain positioning tolerances around h_{opt} , yet the positive and negative tolerances are notably asymmetric. This asymmetry arises because the two sides of the collection efficiency curve are governed by different physical mechanisms. When h exceeds h_{opt} , the decay of collection efficiency is dominated by the exponential falloff of the nanofiber evanescent field. When h is below h_{opt} , the decay of collection efficiency is constrained by the perturbation of the waveguide mode induced by the bulk material with a high refractive index. Next, we study the effect of the color center depth D on the collection efficiency η .

The depth of the color center (D) within the bulk material is another key parameter affecting η , as the optical properties of the color center are highly contingent upon its local environment. Taking the NV center as an example, when it is located closer to the diamond surface, the NV center's fluorescence experiences less suppression from total internal reflection. This reduction allows for more efficient collection of the fluorescence emitted by the color center, despite the increased susceptibility to surface-related perturbations such as surface spins and impurity electrons. To investigate the dependence of η on D , the values of h and d are set to the optimal values based on the results from Fig. 4. The optimal parameters h and d are 180 nm and 850 nm for the V_{Si} in 4H-SiC, and 140 nm and 650 nm for the NV center in diamond, respectively. Figure 5 illustrates the dependence of η on D , varied from 0 nm to 1000 nm. The simulation results for the V_{Si} in 4H-SiC and the NV center in diamond are presented in Fig. 5 (a) and (b), respectively. The maximum η occurs when the color center is located at the surface of the bulk material ($D = 0$ nm). For $D < 50$ nm, η decreases sharply with increasing D . Beyond $D = 50$ nm, η continues to decline gradually with small fluctuations. This trend is physically consistent with the exponential decay of the near-field component of the dipole radiation field at the top surface of the bulk material as D increases. In the limit of infinite D , the evanescent field intensity at the top surface would approach zero, and η should theoretically tend to zero. However, within the finite depth range investigated, the attenuation is limited, and η exhibits a gradual decreasing trend rather than a sharp drop to zero. The minor fluctuations are likely caused by inter-

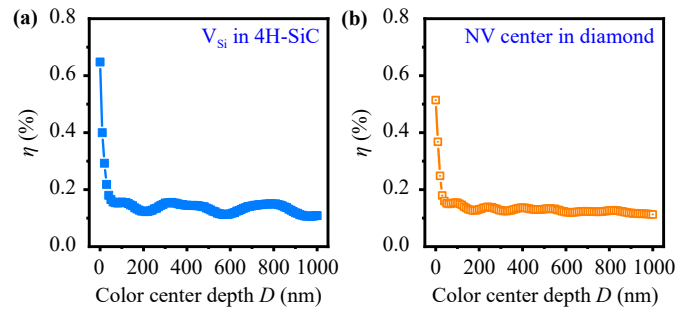


Fig. 5 Collection efficiency η as a function of D for (a) the V_{Si} in 4H-SiC and (b) the NV center in diamond. The parameters h and d are set to the optimal values from Fig. 4 for each color center: 180 nm and 850 nm for the V_{Si} in 4H-SiC, and 140 nm and 650 nm for the NV center in diamond. The highest collection efficiency occurs at the surface ($D = 0$ nm). Over the simulation range of 0–1000 nm, η decreases sharply for $D < 50$ nm, followed by a gradual decline superimposed with small non-monotonic fluctuations at larger depths.

ference effects between the nanofiber evanescent field and the color center radiation field, mode-dependent coupling variations in the multimode nanofiber, or numerical artifacts from finite mesh resolution and residual PML absorption, but they do not affect the main conclusions. Consequently, shallow implantation is typically employed to place color centers near the surface. This facilitates the applications of microwave, radio-frequency and optical control fields, enabling more efficient and precise initialization, manipulation, and readout of the spin qubits [47, 52].

Finally, the effective spatial response of a nanofiber along the y -axis is simulated by varying the transverse distance between the color center and the nanofiber. To quantify this, we adapt the model in Fig. 1 for a V_{Si} in 4H-SiC. The simulation employs a nanofiber of diameter $d = 400$ nm, with the color center at a depth $D = 30$ nm and the previously determined optimal distance $h = 420$ nm. The y -coordinate of the nanofiber is varied from -1000 nm to 1000 nm, where $y = 0$ nm defines its position directly above the color center.

The simulation results are solid purple squares shown in Fig. 6, which is fitted with Lorentzian function (solid dark purple curve). The full width at half maximum (FWHM) is 853 ± 9 nm. This FWHM defines the effective spatial response of the nanofiber along the y -axis for color center detection, representing the coupling range of the nanofiber's evanescent field. To substantiate the physical basis of the Lorentzian fitting, we extract normalized y -directional profiles at the color-center depth for both the intrinsic HE_{11} mode field of the nanofiber and the interaction field between the nanofiber and the bulk material, as shown in Fig. 6(b). The Lorentzian function reproduces the simulated data excellently across the full transverse range, particularly in the

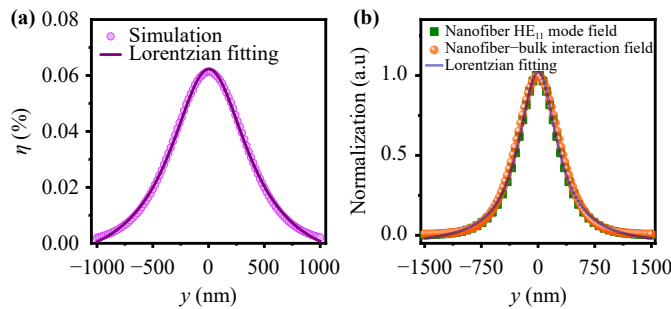


Fig. 6 (a) Effective spatial response of the nanofiber along the y axis for V_{Si} in 4H-SiC. The collection efficiency η is plotted as a function of the nanofiber's y -coordinate. Purple solid squares represent simulation results, and the dark purple solid curve shows the corresponding Lorentzian fit with a FWHM of 853 ± 9 nm. (b) Normalized one-dimensional y -directional field profiles at the color-center depth for the intrinsic HE_{11} mode field of the nanofiber and the interaction field between the nanofiber and the bulk material, both fitted with Lorentzian functions. Green squares denote the intrinsic HE_{11} mode field of the nanofiber, orange circles denote the interface-modified mode field near the bulk material, and light blue curves represent the corresponding Lorentzian fits. All profiles are normalized to their respective peak values. Simulation parameters for both panels: nanofiber diameter $d = 400$ nm, V_{Si} depth $D = 30$ nm, and optimal nanofiber-bulk distance $h = 420$ nm.

tail regions, whereas the Gaussian fit exhibits substantial deviations, as detailed in appendix. This provides a physical justification for the Lorentzian fitting employed in Fig. 6(a). For the highly sensitive defect detection needed in quantum technology applications [12–19], the effective spatial response achieved in this model may still require improvement. One viable approach is to reduce the nanofiber diameter. The above analysis indicates that the proposed scheme has achieved clear performance metrics in terms of collection efficiency and probing width, although several aspects still require further optimization.

A quantitative comparison between the proposed scheme and existing fluorescence collection techniques is as follows. Confocal microscopy with an $NA = 0.95$ air objective achieves a collection efficiency of about 3%; even with an $NA = 1.49$ oil immersion objective, the efficiency remains only about 10% [20]. Its spatial resolution is limited by the diffraction limit. Its spatial resolution is limited by the diffraction limit. According to the Rayleigh criterion, for 637 nm fluorescence the transverse spatial resolutions for $NA = 0.95$ and $NA = 1.49$ objectives are approximately 409 nm and 261 nm, respectively; for 917 nm fluorescence they are approximately 590 nm and 375 nm, respectively. Moreover, confocal microscopy systems are bulky, costly, and the immersion oil contaminates the bulk. Solid immersion lenses can improve the collection efficiency to 20%–30%, but their spatial resolution is constrained by their physical dimensions, typically

exceeding 1 μm , and their fabrication is invasive and requires precise alignment with individual color centers [21]. Monolithic immersion metalenses can enhance fluorescence collection efficiency to $\sim 35\%$, yet their spatial resolution is limited by the metasurface aperture and nanopillar dimensions, with a diffraction-limited resolution of about 388 nm [22]. Furthermore, their fabrication involves complex electron-beam lithography and dry etching processes, making them costly and unsuitable for high-throughput production. Microdisk resonators and nanopillars also enhance collection efficiency, but their fluorescence signals still rely on an objective for collection, and the fabrication processes are complex and costly [23–26]. Waveguide-integrated color centers with photonic crystal reflectors show potential for efficient readout, but the overall system still depends on complex micro/nano fabrication and is invasive to bulk materials [27]. It should be noted that the objective and the nanofiber rely on fundamentally different physical mechanisms. The objective collects far-field propagating waves that escape the bulk-air interface and enter its collection solid angle, whereas the nanofiber collects fluorescence through near-field evanescent-wave coupling into its guided modes. For a rigorous comparison, both collection efficiencies are normalized to the total radiated power of the same color center in the bulk material, and the comparison is made at the first collection stage. Following the calculation method in the supplementary material of Ref. [20], under identical conditions, namely an NV center in bulk diamond at a depth of 30 nm with an emission wavelength of 637 nm, the estimated collection efficiency of confocal microscopy is about 2.77%. In comparison, this work achieves a peak collection efficiency of 0.18% for the NV center in diamond. Although the simulated fluorescence collection efficiency is lower than that of conventional free-space detection schemes, the proposed scheme offers unique advantages, including non-invasiveness, integrability, low cost, objective-free operation, and inherent compatibility with single-mode fiber systems through adiabatic tapering, making it well-suited for high-throughput, in-situ, and rapid characterization.

We further analyze the rationality of the idealized simulation model and its experimental feasibility. The nanofiber is modeled as a straight cylindrical waveguide in simulations, which fully corresponds to the uniform waist region of the silica nanofibers fabricated in our laboratory. This waist region features a uniform diameter, smooth surface and a length of approximately 2 mm, highly consistent with the geometric settings of the simulation model. Even when a bent nanofiber is adopted to avoid direct contact with the bulk sample, the local coupling segment within the interaction region can still be approximated as a straight waveguide [53], and the model conclusions remain applicable. The model assumes a flat surface of the bulk material. Although



surface roughness, surface defects, substrate background fluorescence and interfacial scattering of actual bulks exert certain effects on the collection efficiency, they only cause minor corrections to the absolute value of efficiency and do not alter the qualitative conclusions obtained in this work. Specifically, surface roughness induces scattering loss and local spacing fluctuation, resulting in spatial inhomogeneity of coupling strength. Surface defects reduce the quantum yield of near-surface color centers but do not change the intrinsic distribution of collection efficiency. Substrate background fluorescence and interfacial scattering mainly elevate the background count and degrade the signal-to-noise ratio, which can be effectively suppressed by spectral filtering. Meanwhile, the parallel near-field coupling assumption is well supported by experimental feasibility and mature techniques, and has been widely validated in systems such as planar waveguides [54] and silicon microdisk cavities [55]. In our ongoing experiments, the position and tilt angle of the nanofiber can be precisely controlled via a three-dimensional nano-positioning stage and a dual-axis tilt adjustment platform, enabling stable reproduction of the parallel near-field coupling configuration assumed in the simulation. Finally, the present model targets general bulk materials with unknown crystal orientation, where the transition dipoles of color centers are randomly distributed in three-dimensional space. Accordingly, when calculating the collection efficiency, we perform independent simulations for three orthogonal polarization directions, namely radial, azimuthal and axial, and take their arithmetic mean as the final collection efficiency. This treatment equivalently introduces a virtual longitudinal dipole component, so the collection efficiency obtained in this work serves as a conservative lower bound of the actual value. In summary, all idealized assumptions in the simulation model can be effectively realized in experiments via mature techniques, and the core qualitative conclusions revealed in this work will remain unchanged in experimental validation.

Although the idealized simulation model described above has sound experimental feasibility, the proposed nanofiber-based color center detection scheme still has two intrinsic limitations. First, total internal reflection at the interface between air and the high-refractive-index bulk material traps most of the fluorescence emitted by color centers, and only a small fraction of photons can reach the surface to participate in near-field coupling, which is the primary reason for the relatively low collection efficiency achieved to date. Second, the low refractive index of silica nanofibers results in limited evanescent field intensity and a short effective interaction distance, which constrains further improvement of the collection efficiency. Future optimization can be carried out in two directions, material selection and structural design. In terms of material selection, high refractive index materials such as silicon nitride and titanium

dioxide can be explored to fabricate nanofibers, so as to enhance the evanescent field intensity and improve the spatial overlap between the guided mode and color center emission. In terms of structural design, photonic crystal or Bragg grating structures can be introduced on the nanofiber surface to tailor the mode field distribution and enhance the directional coupling capability [56–59]. The quantitative performance of these optimized structures will be systematically verified through dedicated simulations and experiments in subsequent work, while the non-invasive and integrable advantages of the scheme will be maintained.

4 Conclusions

This paper proposes and theoretically validates a scheme for collecting fluorescence from color centers in bulk materials using the near field of a nanofiber. Based on our three-dimensional FDTD model, we demonstrate that a nanofiber can be used to detect fluorescence from various color centers in bulk materials and quantitatively evaluate the collection efficiency η . We systematically simulate the influence of key parameters on η , including the nanofiber diameter, the distance between the nanofiber and the sample, and the color center depth. Quantitative design rules are provided for two representative color centers, namely the V_{Si} in 4H-SiC and the NV center in diamond. The optimal parameters obtained from simulations are as follows. For the V_{Si} in 4H-SiC, the optimal distance is 180 nm and the optimal diameter is 850 nm, yielding a maximum collection efficiency of 0.22%. For the NV center in diamond, the optimal distance is 140 nm and the optimal diameter is 650 nm, yielding a maximum collection efficiency of 0.18%. Additionally, we simulate the effective spatial response for detecting a V_{Si} in 4H-SiC at a depth of 30 nm using a nanofiber with a diameter of 400 nm, achieving a transverse effective spatial response of 853 ± 9 nm. As discussed in Section 3, compared with existing methods, the proposed scheme, despite its limited fluorescence collection efficiency, offers unique advantages of non-invasiveness, integrability, high throughput, scalability, and compatibility with optical fibers. The scheme exhibits clear experimental feasibility based on mature micro/nano fabrication and precision positioning techniques [50, 60]. Anticipated technical challenges such as mechanical stability and background light suppression can be addressed by vibration isolation, optical filtering, and post-implantation annealing.

These simulation results and performance assessments demonstrate that the nanofiber-based color center detection system has multiple technical advantages and expansion potentials compared with conventional objective-based schemes. The scheme is highly scalable and

can be adapted to various color center systems in different host materials by optimizing geometric parameters and coupling conditions [2–9]. Different from conventional point-by-point scanning modes, this system supports one-dimensional line detection and can be extended to two-dimensional area scanning, providing a novel technical route for high-throughput defect inspection in semiconductor wafers [19, 57]. The inherent compatibility between nanofibers and commercial single-mode fibers lays the foundation for constructing all-fiber integrated systems integrating color-center fluorescence collection transmission and detection [2, 3, 8–19, 59]. For in-situ detection scenarios in complex devices such as quantum chips [61, 62], this scheme offers a compact and non-invasive solution that breaks through the detection limitations of conventional objectives imposed by spatial and working distance constraints. Furthermore, the fluorescence collection efficiency of the system still has considerable room for improvement. Future work will focus on enhancing evanescent field coupling via higher-refractive-index nanofibers, and realizing directional collection enhancement via photonic micro/nano structures on nanofiber surfaces [56–59]. These application prospects and optimization directions are potential research paths, and their practical realization remains to be validated by dedicated follow-up experiments. In summary, this work provides a new technical route for defect detection in bulk materials, and also offers theoretical guidance and parametric reference for subsequent experimental studies.

Declarations The authors declare that they have no competing interests and there are no conflicts.

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Appendix A: Physical basis for Lorentzian fitting of spatial response

The collection efficiency η versus the color-center lateral position along the y axis (Fig. 6) is fundamentally governed by the mode-field overlap integral between the color-center dipole emission field and the evanescent field of the nanofiber HE_{11} mode. As the color center is displaced laterally away from the nanofiber axis, the variation of this overlap integral follows the spatial decay profile of the evanescent field. To elucidate the

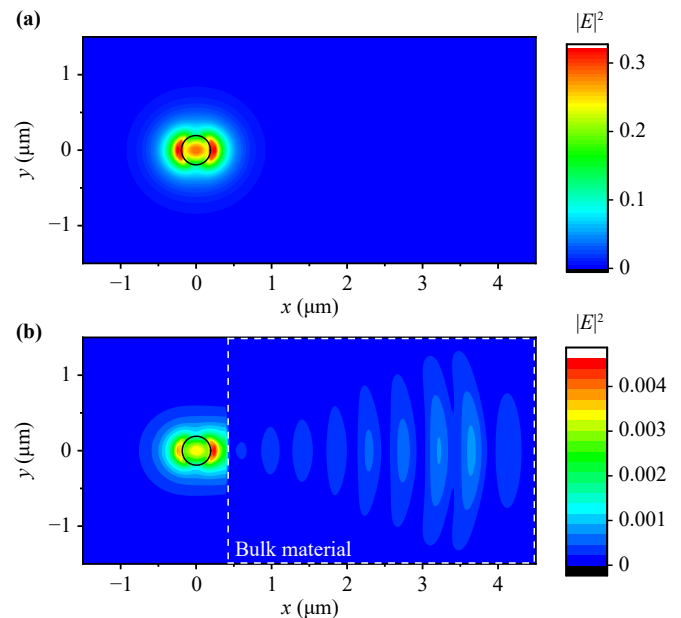


Fig. A1 Transverse (x - y plane) field distributions of the nanofiber HE_{11} mode. (a) Intrinsic HE_{11} mode field of the nanofiber. (b) Field distribution in the presence of the bulk material. The black circle indicates the nanofiber cross section, and the white dashed box outlines the bulk material region. Simulations use the same geometric parameters as Fig. 6 of the main text: 400 nm nanofiber diameter, 30 nm color-center depth, and 420 nm nanofiber–bulk distance.

physical rationale for the Lorentzian fitting adopted in the main text, we perform field distribution simulations with the same parameters as Fig. 6.

Figure A1 shows the spatial distributions of the electric field intensity $|E|^2$ for two configurations. (a) Intrinsic HE_{11} mode field of the nanofiber: the field is predominantly confined within the nanofiber (black circle), with a slowly decaying evanescent field extending radially outward. (b) Field distribution when the nanofiber is adjacent to the bulk material (white dashed box): the high-index bulk modulates the evanescent field at the interface, such that the field penetrates into the bulk with a gradually decaying transverse envelope. This simulation includes no color centers and serves solely to illustrate the influence of the bulk interface on the nanofiber mode field.

To further validate the Lorentzian fitting employed in Fig. 6(a), we perform a direct comparison with Gaussian fitting. Figure A2 presents the Gaussian fits obtained using the same normalized one-dimensional y -directional profiles at the color-center depth as in Fig. 6(b). While the Gaussian function yields a reasonable fit near the peak, it decays substantially faster than the simulated field distribution in the tail regions, resulting in clear deviations from the data. This comparison corroborates the choice of the Lorentzian function in Fig. 6(a).

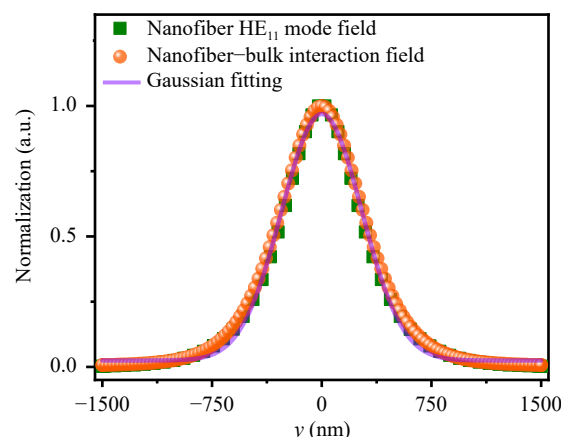


Fig. A2 Normalized one-dimensional y -directional profiles at the color-center depth, derived from the same dataset as Fig. 6(b) and fitted with Gaussian functions. Green squares denote the intrinsic HE_{11} mode field of the nanofiber, orange circles denote the interface-modulated mode field near the bulk material, and light purple curves represent the corresponding Gaussian fits. All profiles are normalized to their respective peak values.

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