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Quality factor enhancement of spherical resonators by radial anisotropy

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Abstract. High-quality resonances in open systems have ubiquitous applications in nanophotonics. However, it is challenging to achieve high quality factor in compact resonators due to the limitations on the refractive index of materials. Recently a novel family of high index materials was discovered, i.e., van der Waals materials. In addition to record-high refractive indices, they feature strong negative optical anisotropy, therefore their promise for the use in nanoresonators is not evident. Motivated by the progress in fabrication of spherical nanoparticles from these materials, here we study the effect of radial anisotropy on the quality of homogeneous nanospheres that support the Mie resonances. Our study reveals that material anisotropy can enhance the quality factor of Mie resonances. In particular, we show that the quality factor of electric dipole mode of the nanosphere made of radially anisotropic material is up to 29% higher than that of the optically isotropic nanosphere which has the same refractive index.

Keywords: nanoresonators, nanoparticles, van der Waals materials, giant optical anisotropy, Mie resonance

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Материалы конференции
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Повышение добротности сферических резонаторов с помощью радиальной анизотропии

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Аннотация. В данной работе выполнено исследование влияния оптической анизотропии на добротность Ми резонансов сферических наночастиц. Показано, что добротность электрической дипольной моды наносферы из радиально анизотропного материала может превышать добрость аналогичной моды изотропной наносферы до 29%.

Ключевые слова: нанорезонаторы, наночастицы, ван-дер-ваальсовы материалы, гигантская оптическая анизотропия

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Introduction

Light confinement is a topic of great significance in the field of nanophotonics due to its wide-ranging applications [1–3]. Nanoresonators with high quality factors (Q-factors) are suitable for light confinement with a sufficient lifetime in a small volume. Such resonators can enhance the performance of various optical devices such as lasers [4], optical sensors [5] and solar cells [6]. The use of metallic cladding or high-refractive index dielectric materials can enhance the quality factor of compact nanoresonators. However, the use of metal leads to the intrinsic ohmic losses and the Q-factor of high-index dielectric Mie nanoresonators remains small due to the limitations on the refractive index of the materials, so alternative approaches are in high demand.

Our proposed solution in this study utilizes optical anisotropy. To ensure pure Mie resonances, it is crucial to maintain spherical symmetry within the resonator. Therefore, our focus is solely on examining the impact of radial anisotropy on the quality factor. By comparing the results, we observe that negative anisotropy increases the Q-factor even though it decreases the effective refractive index inside the anisotropic medium. Fortunately, transition metal dichalcogenides (TMDC) possess a remarkable ability to exhibit giant negative anisotropy [7], and there have been successful endeavors to fabricate spherical nanoparticles, which feature onion-like crystalline structure and, consequently, radially anisotropic dielectric permittivity tensor [8]. Our findings hold significant potential for the design of Mie resonators with high Q-factors. Also, we provide a tentative physical explanation of the counter-intuitive increase of Q-factor by strong negative anisotropy.

Materials and Methods

The complex eigenfrequencies $\omega = \omega' + i\omega''$ of the electric dipole (ED) resonances were found as poles of ED contribution to the scattering cross-section [9]. For calculations of the scattering cross-section at real and complex frequencies, we employed the spherical transfer matrix method [10] with the necessary adaptations to describe media with radially anisotropic optical response [11]. Finally, to calculate the quality factor of an eigenmode, we used:

$$Q = \frac{\omega'}{2|\omega''|}. \tag{1}$$

Our tentative explanations employ the notion of effective refractive index. Typically, for uniaxial media with a dielectric tensor $\varepsilon = \mathrm{diag}\,(\varepsilon_{||}, \varepsilon_{||}, \varepsilon_{\perp})$, this index is defined as

$$n_{eff}^{p} = \frac{\beta}{\beta_0} = \sqrt{\frac{\varepsilon_{\wedge}\varepsilon_{P}}{\varepsilon_{P}\sin^2\theta_1 + \varepsilon_{\wedge}\cos^2\theta_1}}, \tag{2}$$

where β and β_0 are the wavenumbers of p-polarized wave in the anisotropic medium and in vacuum respectively and θ_1 is the angle between the wavevector of the plane wave and the optical axis. When the refraction at the interface normal to the optical axis is considered, the angle of incidence and refraction obey Snell's law $n_{eff}^{p}\sin\theta_1 = n_2\sin\theta_2$, where n_2 is the refractive index of the adjacent medium and θ_2 is the angle of refraction.

Given these properties, one might expect that amplitude of reflection of p-polarized wave at

the interface is given by the Fresnel equation as $r = \dfrac{n_{eff}^{p} \cos\,\theta_2 - n_2 \cos\,\theta_1}{n_{eff}^{p} \cos\,\theta_2 + n_2 \cos\,\theta_1}$.
However, this statement is wrong, and the reflection amplitude is actually given by [12]:

$$r = \frac{\dfrac{\varepsilon_P}{n_{eff}^{p}} \cos\theta_2 - n_2 \cos\theta_1}{\dfrac{\varepsilon_P}{n_{eff}^{p}} \cos\theta_2 + n_2 \cos\theta_1}. \tag{3}$$

It is evident from Eq. 3 that an "interface-related" effective refractive index should be introduced:

$$n_{eff}^{i} = \varepsilon_P / n_{eff}^{p}. \tag{4}$$

In fact, not only reflection amplitude but the whole transfer-matrix that connects complex amplitudes of plane waves across the interface can be calculated assuming that anisotropic medium is replaced by the isotropic one with a refractive index of n_{eff}^{i} [12]. To distinguish n_{eff}^{i} and n_{eff}^{p}, we will further refer to them as 'propagation-related' and 'interface-related' effective indices.

Results and Discussion

Before the determination of eigenmodes, we calculate ED contribution to the scattering cross-section spectra of homogeneous spheres of radius 100 nm with isotropy Fig. 1, *a* and with negative radial anisotropy Fig. 1, *b*) which would allow us to determine approximate locations and quality of the eigenmodes from resonant peaks. Refractive index n in the isotropic case and the tangential component nt of the refractive index in the anisotropic case were set to 5, which is close to the highest refractive index of transition metal dichalcogenides in their transparency range [13]. For a spherically symmetric structure such as ours, the resonant modes are divided into the transverse-magnetic (TM) modes and the transverse-electric (TE) modes [14, 15]. Since TE modes have no electric field component along the radial direction, they are not affected by the radial anisotropy,

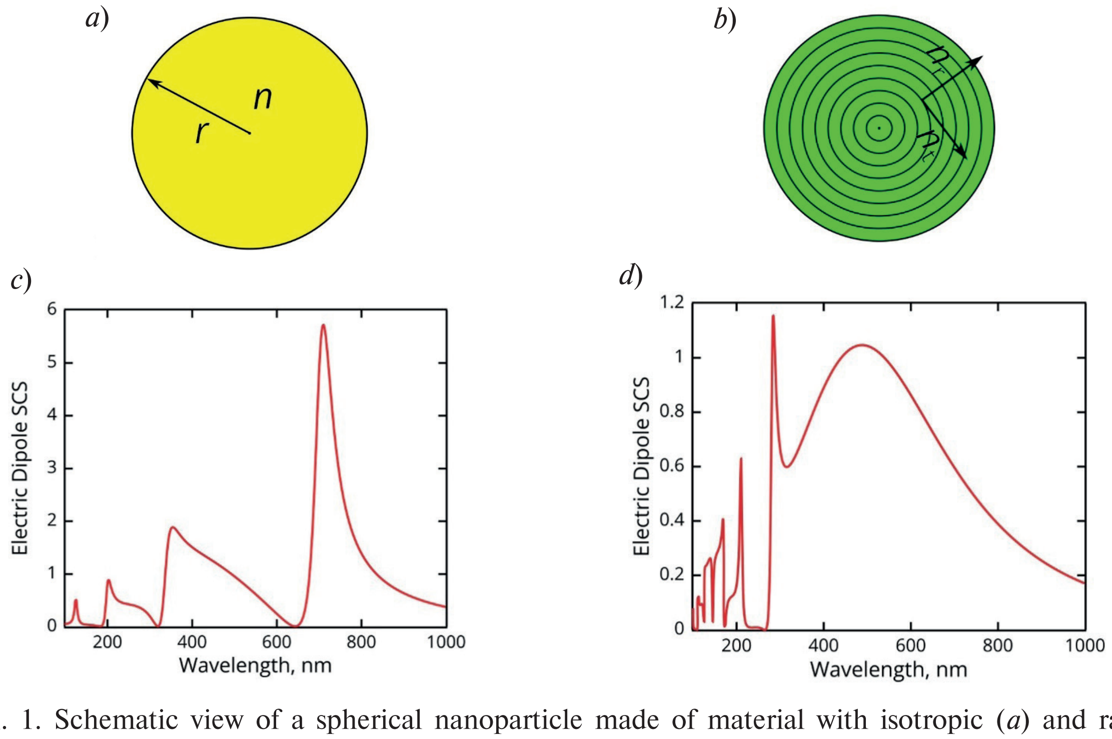

Fig. 1. Schematic view of a spherical nanoparticle made of material with isotropic (*a*) and radially anisotropic (*b*) optical response. Scattering cross-section (SCS) spectra into an eclectic dipole channel for uniform nanoparticles with isotropic (n = 5) (*c*) and radially anisotropic (n_t = 5, n_r = 1) (*d*) optical properties

hence here we studied TM modes only. In particular, we focused on the ED Mie mode since it can be supported by the most compact nanoparticles.

The impact of anisotropy on the resonance frequencies can be observed in Fig. 1 by comparing the scattering cross-section spectra. As we can see, the resonances undergo a blue shift, meaning they are shifted towards shorter wavelengths. The blue shift can be explained by the decreased propagation-related n^p_{eff} by the negative anisotropy as predicted by Eq. 3 and illustrated in Fig. 3, *c*. Such behavior aligns with the isotropic case, where a lower refractive index necessitates photons of greater energy (shorter wavelength) to excite resonance of the same order. At the same time, resonance peaks in the anisotropic case are visibly sharper, which indicates higher quality factor of the corresponding eigenmode.

To gain more understanding of sharper resonances in the anisotropic case, we proceeded with evaluation of the quality factor and the field distribution of the fundamental ED eigenmode (Fig. 2). We varied the radial component of the refractive index from 1 to 10, which allowed us to study the influence of positive and negative optical anisotropy at the same time. We see that positive anisotropy ($n_r > 5$) leads to an increase in the quality factor which may result from the increase in the effective index of waves propagating inside the anisotropic sphere. However, when nr decreases from 5 to 1, the quality factor first decreases, reaching its minimum at $n_r = 2.7$. Subsequently, the quality factor starts to increase again, and at $n_r = 1$, it is 29% higher than the quality factor in the isotropic case ($n_r = 5$) (Fig. 2, *a*). The field distribution in the anisotropic nanoparticle also shows drastic contrast with ED modes in isotropic ones. The maximum of the electric field intensity is observed not in the center. Instead, the electric field is localized in two areas that are close to the surface of the nanosphere (Fig. 2, *b*). We think that this effect is related to large gradients of dielectric permittivity tensor near the center of anisotropic nanosphere.

In isotropic structures, quality factor is known to increase with the refractive index due to the increased momentum mismatch between light inside the resonator and the background [16]. That is why the increase of quality factor with the decrease of radial refractive index appears counterintuitive. To give an intuitive explanation for this phenomenon, we neglected the curvature of the interface between the core and ambient medium and examined the light reflection from planar interface between the isotropic and anisotropic media, as shown schematically in Fig. 3, *a*. The electromagnetic field inside the core can be seen as a superposition of plane waves impinging the interface at different angles. As we found, at a sufficiently strong anisotropy, the reflectance of light incident from the anisotropic medium is greater than that of any incident wave in the isotropic case (see Fig. 3, *b*). The increase in reflectance arises from the fact that the negative anisotropy increases n^i_{eff}, as illustrated in Fig. 3, *c*. As a result, it is more difficult for light to escape from the anisotropic medium which leads to the increase in the quality factor of the ED eigenmode.

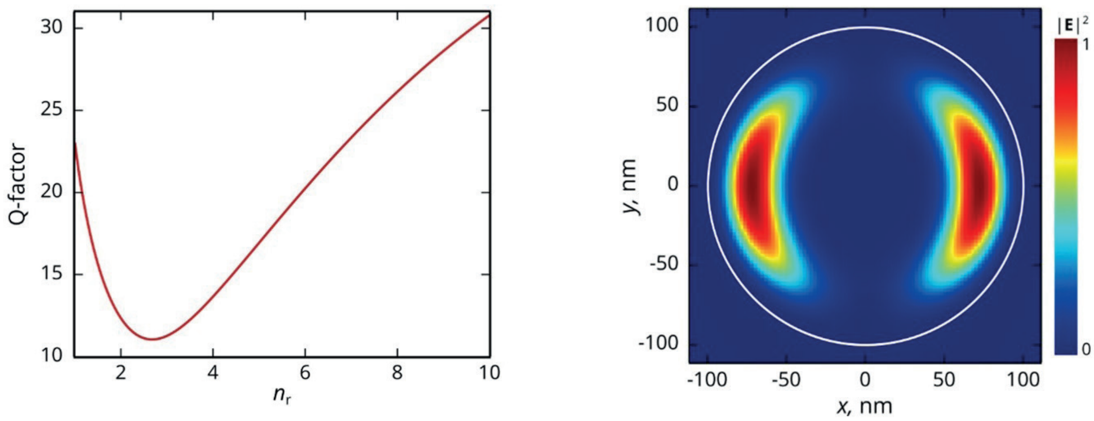

Fig. 2. Quality factor of the ED quasi-normal mode in a radially anisotropic nanosphere as a function of the radial component of the refractive index (*a*). Distribution of the electric field of the mode at $n_t = 5$, $n_r = 1$ (*b*)

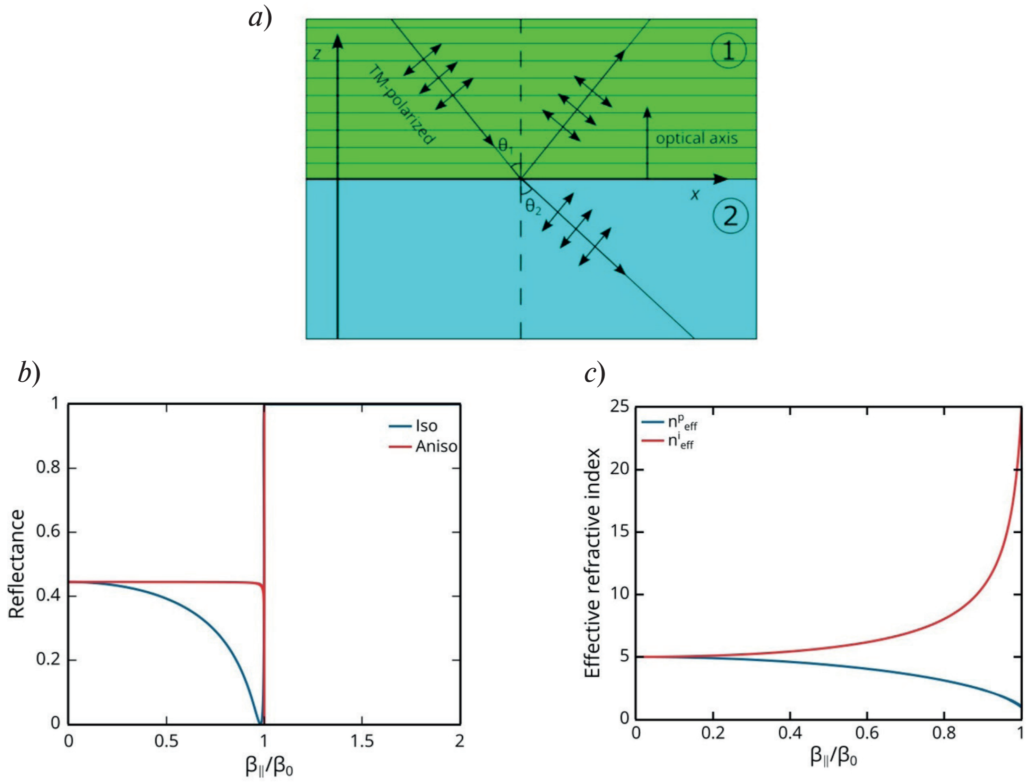

Fig. 3. Schematic representation of a TM-polarized light scattering from the interface of anisotropic and isotropic materials (*a*). Reflectance as a function of β_1/β_0 or anisotropic case (n_t = 5, n_z = 1 and n_2 = 1) and for isotropic case (n_1 = 5 and n_2 = 1) where $\beta_1 = \beta_0 n^p_{eff} \sin\theta_{in}$ is an in-plane component of the wavevector (*b*). Effective refractive indices governing light propagation and interface scattering for the anisotropic medium with n_t = 5, n_z = 1 (*c*)

Conclusion

In conclusion, we studied the impact of radial anisotropy on homogeneous spherical resonators. Our findings revealed that, contrary to expectations, strong negative anisotropy typical for high-index TMDCs can enhance the quality factor of the resonator and produce dramatic changes in the field distribution in the ED mode. Blue shift of the ED mode and increase in the quality factor upon decrease of the radial component of the refractive index are explained by the decrease in the propagation-related refractive index and increase in the interface-related index, correspondingly. Our results show that optical anisotropy, especially the strong optical anisotropy of van der Waals materials, is a promising resource for the efficient light manipulation at the nanoscale.

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