Effective Modal Volume in Nanoscale Photonic and Plasmonic Near-Infrared Resonant Cavities

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Featured Application: A practical guideline to the calculation of effective modal volume for photonic and plasmonic cavities.

Abstract: We survey expressions of the effective modal volume, $V_{\text{eff}}$, commonly used in the literature for nanoscale photonic and plasmonic cavities. We apply different expressions of $V_{\text{eff}}$ to several canonical cavities designed for nanoscale near-infrared light sources, including metallo-dielectric and coaxial geometries. We develop a metric for quantifying the robustness of different $V_{\text{eff}}$ expressions to the different cavities and materials studied. We conclude that no single expression for $V_{\text{eff}}$ is universally applicable. Several expressions yield nearly identical results for cavities with well-confined photonic-type modes. For cavities with poor confinement and a low quality factor, however, expressions using the proper normalization method need to be implemented to adequately describe the diverging behavior of their effective modal volume. The results serve as a practical guideline for mode analysis of nanoscale optical cavities, which show promise for future sensing, communication, and computing platforms.

Keywords: effective modal volume; nanocavities; laser resonators; near-infrared; theory and design

1. Introduction

Semiconductor nanolasers serve simultaneously as a platform for studying intriguing fundamental physics and as a technologically relevant solution for next generation photonic integrated circuits [1,2]. A major drive in the study and application of nanoscale cavities rests in the Purcell effect, which describes the inverse relation between cavity mode volume and the rate of spontaneous emission [3,4]. Smaller cavities generally permit higher rates of spontaneous emission and a greater ratio of spontaneous emission channeled into the lasing mode, which, in principle, provides increased modulation bandwidths and lower lasing thresholds [5,6]. In many nanoscale structures, however, the physical volume of the cavity does not reflect the volume of the cavity mode. Therefore, the effective modal volume, $V_{\text{eff}}$—a unitless quantity normalized with respect to $(\lambda_0/n_a)^3$, was introduced to account for this discrepancy [7]. A complementary expression, the confinement factor, $\Gamma$, may be defined to express the ratio of the volume of the active region, $V_a$, to $V_{\text{eff}}$, namely [8].

$$\Gamma \equiv \frac{V_a}{V_{\text{eff}}}$$

(1)
In purely dielectric cavities with a large physical volume with respect to the cubic wavelength, \( \Gamma \approx 1 \) because the mode is completely confined to the active region. As the active region volume approaches the diffraction limit (approximately given by \( (\lambda_0 / (2n_a))^3 \), where \( \lambda_0 \) and \( n_a \) are the vacuum wavelength and the real part of the active region refractive index, respectively), the cavity mode becomes less confined and \( \Gamma < 1 \). Eventually, when \( V_a / (\lambda_0 / (2n_a))^3 < 1 \), modes are no longer supported in the purely dielectric cavity of which the physical size is below the diffraction limit in all three dimensions. To continue reducing cavity volume, the incorporation of metals becomes inevitable [9]. The plasmonic modes supported by metal–dielectric interfaces in such cavities exhibit considerably different modal profiles from their dielectric counterparts. Namely a substantial portion of modal energy rests at the metal-dielectric interface rather than in the center of a purely dielectric region.

Calculation of \( V_{\text{eff}} \) in three-dimensional (3D) cavities generally requires use of numerical methods due to the geometric and material complexity of the cavities. Physically, the cavity mode is a spatial distribution of electromagnetic energy [10]. Therefore, the calculation essentially requires a comparison of integration of the electromagnetic energy density over the active region domain, \( U_\alpha \), to the integration of the energy density over the entire simulation domain, \( U \). If the simulation domain consists only of dielectric materials, then this calculation is straightforward, and can be expressed as:

\[
\Gamma = \frac{\sum E_{\alpha} + \sum m \alpha}{\sum E_{\alpha}}
\]

\[
= \frac{\int_V d^3r U_\alpha(r) + \int_V d^3r U_m(r)}{\int_V d^3r U_\alpha(r) + \int_V d^3r U_m(r)}
\]

(2)

where \( \Xi \) is the energy, \( r \) is the position vector, and the \( e \), \( m \), and \( a \) subscripts refer to electrical energy, magnetic energy, and active region respectively. For a simulation of non-absorbing and non-dispersive materials, the stored electrical and magnetic energy are identical [11]. Hence, Equation (2) may be simplified to its more commonly seen form of:

\[
\Gamma = \frac{\Xi_\alpha}{\Xi_\alpha + \Xi m \alpha}
\]

\[
= \frac{\int_V d^3r U_\alpha(r)}{\int_V d^3r U_\alpha(r) + \int_V d^3r U_m(r)}
\]

(3)

where \( D \) and \( E \) are the displacement and electric field vectors, respectively (* denotes the conjugated form of the electric field, therefore, the inner product would be the norm of the electric field), \( \Phi_0 \) is the permittivity in vacuum, and \( \varepsilon_r = \varepsilon_R + i\varepsilon_I \) is the, generally, complex valued relative permittivity, with the \( R \) and \( I \) subscripts denoting the real and imaginary part, respectively. In the last equality, \( \alpha \) represents each unique material domain in the simulation over which volume integration must be executed, with the total energy being the sum over these domains. For the study presented in the proceeding sections, we will consider only non-magnetic materials and therefore use Equation (3) as our reference point.

For sake of clarity, we define a material as dielectric or metallic at a given wavelength when \( \varepsilon_R > 0 \) and \( \varepsilon_R < 0 \), respectively. Hence, the same “material” can behave as both dielectric and metal if the simulation includes dispersion over the range of wavelengths in which \( \varepsilon_R \) changes sign. Also, we define a material as absorptive at a given wavelength when \( \varepsilon_I < 0 \) (the negative sign is used to be in accordance with the expression in our simulation software, COMSOL Multiphysics® 5.3 (Burlington, MA, USA)). As most dielectric materials show very weak dispersion and absorption property in the optical regime, if all materials are dielectric, the evaluation of Equation (3) is straightforward, as all of
the terms are positive. If some materials are metallic, but the mode is confined primarily to a dielectric region, Equation (3) remains useful because the denominator remains positive and the small amount of energy contribution from the metallic region introduces only negligible errors in the calculation. However, for cavities supporting surface plasmon polariton (SPP) modes or localized surface plasmon resonance (LSPR) modes where the electric field is strongly confined at the metal–dielectric interface, the amount of energy stored and dissipated by metal is no longer negligible. Equation (3) becomes invalid because the resulting negative energy has no physical meaning.

To circumvent this problem, the real part of the permittivity in Equation (3) can be replaced by an average permittivity, defined as [12]. As $\omega \gg \gamma$ (damping constant) in most of the optical applications, both $\varepsilon_g$ and $(\varepsilon_g(\omega) + \varepsilon_R(\omega))/2$ are positive.

$$\varepsilon_{\text{avg}}(r, \omega) = \frac{(\varepsilon_g(r, \omega) + \varepsilon_R(r, \omega))}{2} \quad (4)$$

where $\omega$ is the angular frequency, related to the vacuum wavelength via the vacuum speed of light, $c$, by $\omega = 2\pi c/\lambda_0$, and $\varepsilon_g$ is the group permittivity. The latter is calculated as:

$$\varepsilon_g = \frac{\partial[\omega\varepsilon_R(r, \omega)]}{\partial\omega} \quad (5)$$

Use of Equation (4) in place of simply $\varepsilon_r$ accounts for the physical effects of dispersion and usually ensures mathematically that the all the terms in the denominator of Equation (3) will be positive because in most cases $\varepsilon_g + \varepsilon_R > 0$. For example, use of the Drude model for the complex permittivity of gold (Au) leads to $\varepsilon_g + \varepsilon_R > 0$ [12]. However, use of experimental data [13] for the permittivity of Ag may lead to $\varepsilon_g + \varepsilon_R < 0$, such that $\varepsilon_{\text{avg}} < 0$. In this case, use of $\varepsilon_r$ in Equation (3) may be replaced directly by Equation (5), which will always be positive [14–16].

Despite the circumvention of the failure of Equation (3) via Equations (4) and (5), a number of different expressions for the effective modal volume have appeared in the literature [17–21]. It is the purpose of this paper to assess the utility of these expressions for the design and analysis of nanoscale photonic and plasmonic cavities. For concreteness, we evaluate the expressions for near-infrared (IR) resonant cavities. In Table 1, we list all three different nanoscale cavities we have evaluated, and categorize them according to the optical mode they support. Therefore, we provide a practical guideline on how to implement each effective modal expression. It should be understood, however, that our approach could be applied to cavities supporting modes at other frequencies as well.

| Table 1. Mode features of investigated nanoscale cavities. (AZO: aluminum-doped zinc oxide.) |
|---------------------------------------------------------------|
| **Metallo–Dielectric Cavity with Ag** | **Metallic Coaxial Cavity with AZO** | **Metallic Coaxial Cavity with Ag** |
| Photonic Mode | x | x | |
| Plasmonic Mode | | x | |
| Confined Mode | x | x | |
| Leaky Mode | x | x | |

The paper is organized as follows. In Section 2 we expand upon the introduction and review the various expressions for $V_{\text{eff}}$ found in the literature. Next, in Section 3 we apply these expressions to several canonical cavity geometries, including a metallo-dielectric cavity that supports photonic modes [22] and a coaxial cavity that supports plasmonic modes [6]. In all cases, indium gallium arsenide phosphate (InGaAsP) serves as the active region material, with alloy composition chosen such that emission occurs in the wavelength range of $1260 \text{ nm} < \lambda_0 < 1590 \text{ nm}$. For the coaxial geometry, we study both Ag and aluminum-doped zinc oxide (AZO) as the cladding materials, whereas only Ag is used for the metallo–dielectric geometry. The plasma frequency of Ag and AZO lie in the
ultraviolet and near-IR wavelengths, respectively, with the latter being tunable depending on its alloy composition [23]. Therefore, we compare cases when the active material emission frequency and the cavity resonance frequency are far from and close to the plasma frequency of the constituent metal. Room temperature conditions are assumed for all calculations and values of permittivity are taken from the literature [23–25]. It should be emphasized that in calculating $V_{eff}$, we include both the real and imaginary parts of the metal permittivity to account for realistic absorption losses. However, we use only the real part of the InGaAsP permittivity because we are primarily interested in the degree to which electromagnetic energy may be stored in the active region. When considering absorption or amplification of energy in the active region, the numerator of Equation (3) can be used with the substitution of $\varepsilon_I$ for $\varepsilon_r$, which has been theoretically proved and verified by numerical simulation, respectively [26,27]. In Section 4, we discuss our results and present a metric for comparing the robustness of the various expressions. We conclude the paper in Section 5.

2. Materials and Methods

In this section, we present five expressions for $V_{eff}$ from the literature. The first expression, $V_{eff,1}$, was presented for use in a photonic crystal cavity with an air gap and containing only dielectric materials [17]. It is:

$$V_{eff,1} = \frac{\sum_\alpha \int_{V_{\alpha}} d^3r_{\alpha} \left( \varepsilon_{\alpha}(r_{\alpha}) |E_{\alpha}(r_{\alpha})|^2 \right)}{\varepsilon(\mathbf{r}_{\max}) \max(|E(\mathbf{r}_{\max})|)^2}$$  (6)

The denominator of Equation (6) includes the maximum of the electric field, where $r_{\max}$ denotes the position of electric field antinode. Additionally, the permittivity of the denominator equals that of the material in which the maximum electric field antinode is located.

The second expression, $V_{eff,2}$, was used in the analysis of metallic nanocube antennas [18]. It defines the effective volume as the ratio of total electrical energy to the peak value of electrical energy density. Using the earlier introduced notation:

$$V_{eff,2} = \frac{\sum_\alpha \int_{V_{\alpha}} d^3r_{\alpha} \left( \varepsilon_{\alpha}(r_{\alpha}) |E_{\alpha}(r_{\alpha})|^2 \right)}{\varepsilon(\mathbf{r}_{\max}) \max(|E(\mathbf{r}_{\max})|)^2}$$  (7)

If the peak energy density is located in the active region, then Equation (7) leads to the reference expression for $\Gamma$, i.e., Equation (3), after division by $V_a$. If the peak electric field lies in the active region, then Equations (6) and (7) yield the same result. However, in some geometries, the peak electric field could reside in a low index region, such as an air gap, while the peak energy density lies in the high index active region, in which case Equations (6) and (7) will yield different results.

The third effective volume expression, $V_{eff,3}$, was used in the analysis of spontaneous emission enhancement in a dielectric pillar microcavity [19] and a metallo–dielectric cavity [22]. It is:

$$V_{eff,3} = \frac{\sum_\alpha \int_{V_{\alpha}} d^3r_{\alpha} \left( n_{\alpha}(r_{\alpha})^2 |f_{\alpha}(r_{\alpha})|^2 \right)}{n_a^2}$$  (8)

where $f$ is the normalized electric field such that $|f(\mathbf{r})| = 1$ at the field antinode. While Equation (8) appears to differ from Equations (6) and (7) in that the electric field is absent from the denominator, the normalization effectively supplies the electric field to both the numerator and denominator. If all materials in the cavity are lossless dielectric and the peak electric field resides in the active region, then $V_{eff,3}$ yields identical results to $V_{eff,2}$ and $V_{eff,1}$. However the use of the active region refractive index in the denominator of Equation (8), regardless of the location of peak field or energy, generally leads to values of $V_{eff,3}$ different from $V_{eff,1}$ and $V_{eff,2}$.
The fourth effective volume expression that we assess, $V_{eff4}$, is \cite{20,28,29}:

$$V_{eff4} = \left( \frac{1}{V_p^4} \right)^{-1}$$  \hspace{1cm} (9)

where $V_p$ is defined as:

$$V_p = \sum \left( \int \sigma d^3 r \frac{E_\alpha(r_\alpha)}{E_\alpha(r_\alpha)^2} \right) = \left[ \frac{\varepsilon_{max}(E_{max})}{\sum \left( \int \sigma d^3 r \frac{E_\alpha(r_\alpha)}{E_\alpha(r_\alpha)^2} \right)} \right]^{-1}$$

For $V_{eff4}$, $\varepsilon_\alpha$ is replaced by $\sigma$ according to the normalization method that has been introduced \cite{28}, where, $\tilde{\omega}_c$ refers to the complex eigenfrequency of the cavity mode, and $\varepsilon_B$ refers to the relative permittivity of the background material surrounding the cavity or resonator.

$$\sigma = \frac{1}{2\tilde{\omega}_c} \frac{\partial [\varepsilon_\alpha(r, \tilde{\omega}_c)]}{\partial \tilde{\omega}_c}$$  \hspace{1cm} (11)

If the mode is well confined to the center of the cavity, then the field will converge to zero at the edge of the simulation domain and the second term in the numerator surface integration term of Equation (10) becomes negligible. In this case, Equation (10) becomes:

$$V_{eff4} \approx \left[ \frac{\varepsilon_{max}(E_{max})}{\sum \left( \int \sigma d^3 r \frac{E_\alpha(r_\alpha)}{E_\alpha(r_\alpha)^2} \right)} \right]^{-1}$$

For a well confined cavity, the quality factor (Q factor) is usually high, therefore, $\tilde{\omega}_c/\omega_c \approx 1$. Then, $V_{eff4}$ is identical to Equation (6) of $V_{eff1}$. It should be noted that the convergence of $V_{eff4}$ is based on the usage of complex eigenfrequency and unconjugated inner product of the electric field \cite{28}.

The fifth and final effective volume expression that we assess, $V_{eff5}$, is \cite{21,30–32}:

$$V_{eff5} = \left( \frac{1}{V_q^4} \right)^{-1}$$  \hspace{1cm} (13)
where $V_q$ is defined as:

$$
V_q \equiv \sum_{\alpha} \left( \int_V \varepsilon_{\alpha \varepsilon_c} \varepsilon_{\gamma_c} \left( \int_V \varepsilon_{\alpha \varepsilon_c} \varepsilon_{\gamma_c} (r) E_{\alpha}^2 \varepsilon_{\gamma_c} (r) \right) \varepsilon_{\gamma_c} (r) \max \left( E(r) \right)^2 \right) + \int_{V_{\text{PML}}} \varepsilon_{\gamma_c} (r) \max \left( E(r) \right)^2 \varepsilon_{\gamma_c} (r) \max \left( E(r) \right)^2
$$

(14)

For $V_{\text{eff},5}$, $\varepsilon_r$ is replaced by $\varepsilon_{\gamma_c}$, where ‘gc’ stands for a complex group permittivity [21].

$$
\varepsilon_{\gamma_c} = \varepsilon_r + \frac{\partial \left[ \tilde{\omega}_c \varepsilon_r (r, \tilde{\omega}_c) \right]}{\partial \tilde{\omega}_c}
$$

(15)

In $V_{\text{eff},5}$, the surface integration term in Equation (10) is replaced by the integration of energy density in the perfectly matched layer (PML) in the simulation domain. As $E(r)$ exponentially diverges in space when $|r| \to \infty$, a leaky mode cannot be readily normalized with energy consideration based merely on the conjugated form of the electric field inner product $E(r) \cdot E(r)^*$, which is the modulus square of the electric field used in $V_{\text{eff},1,2,3}$. To include the impact of absorption and/or radiation loss, which is embedded in $\text{Im}(E)$, the unconjugated form $E(r) \cdot E(r)$ needs to be used for leaky cavities. The formulae of $V_{\text{eff},4}$ and $V_{\text{eff},5}$ are both based on this energy consideration of the unconjugated form $E(r) \cdot E(r)$, therefore, theoretically, these last two effective modal volume expression yield more accurate $V_{\text{eff}}$ value for cavities with significant amount of absorption and/or radiation loss. Comparing $V_{\text{eff},4}$ and $V_{\text{eff},5}$, $V_{\text{eff},4}$ requires a surface integration of electric energy density over the boundary of a large simulation domain, which may constrain its applicability for users with limited physical memory of their computation tool. The physical memory requirement for eigenfrequency study in COMSOL grows linearly with the increase in degree of freedom and meshing elements; therefore, there exists an upper limit for simulation domain size. On the other hand, $V_{\text{eff},5}$ requires the knowledge of the exact permittivity and permeability distributions in the PML, which may not be possible in all commercial software [30]. Nevertheless, the normalization condition of $V_{\text{eff},5}$ can be easily extended for dispersive and magnetic materials.

To simulate these three different cavities, eigenfrequency study is performed with the Wave Optics module in the commercial finite element method (FEM) software COMSOL. The cavities are enclosed with spherical shape background material and perfectly match layer (PML). The detailed meshing conditions are listed in Table 2, where $\lambda_L$ is 1.26 µm, corresponding to the lower edge of InGaAsP quantum well gain spectrum at room temperature; $n_{\text{InGaAsP}}$ and $n_{\text{air}}$ are refractive indices of InGaAsP and air, respectively.

| PML | Fine | Normal |
|-----|------|--------|
| Number of layers | 10 | 5 |
| Cavity Type | Free tetrahedral (extremely fine) | Free tetrahedral (fine) |
| Maximum element size (nm) | $\lambda_L/(6 \cdot n_{\text{InGaAsP}})$ | $\lambda_L/(4 \cdot n_{\text{InGaAsP}})$ |
| Background Type | Free tetrahedral (normal) | Free tetrahedral (normal) |
| Maximum element size (nm) | $\lambda_L/(6 \cdot n_{\text{air}})$ | $\lambda_L/(4 \cdot n_{\text{air}})$ |
| Metal-dielectric boundary Type | Free tetrahedral (extremely fine) | Free tetrahedral (extra fine) |
| Maximum element size (nm) | 10 | 20 |
3. Results

3.1. Metallo-Dielectric Resonator

We first present results on the evaluation of different $V_{\text{eff}}$ expressions for the Ag-cladded metallo–dielectric cavity. As the dielectric ($\text{SiO}_2$) cladding (200 nm) between cavity core (InGaAsP) and cavity shell (Ag) is thick enough, the cavity supports well confined photonic modes, and the electric fields outside the active region quickly converge to zero. Therefore, we anticipate minor variation in the resulting $V_{\text{eff}}$ values with respect to change of simulation domain size ($d_{\text{air}}$) compared to cavities supporting leaky plasmonic modes, such as those in Sections 3.2 and 3.3.

Figure 1. (a) Closeup of the transverse electric (TE) $\text{TE}_{012}$ mode in the metallo–dielectric cavity (lengths expressed in nm) (b) Entire simulation space for the metallo–dielectric cavity (c) $V_{\text{eff}}$ as a function of $d_{\text{air}}$ evaluated for the various expressions. All of the traces overlap. ($Q = 2700.8$ at $2.0169\times10^{14}$ Hz ($\lambda_0 = 1486.4$ nm)).

A cross section of the metallo–dielectric cavity is shown in Figure 1a, where $|E(r)|$ of the $\text{TE}_{012}$ mode is plotted. It is apparent that the optical mode mostly overlaps with the InGaAsP active region. Further, because the ratio of relative permittivity of InGaAsP to $\text{SiO}_2$ is $(n_{\text{InGaAsP}}/n_{\text{SiO}_2})^2 \approx (3.4/1.45)^2 = 5.5$, the concentration of energy in the active region can be found by scaling the color plot of Figure 1a by a magnification factor of 5.5. This will lead to a confinement factor as given by Equation (3) close to unity. The simulation domain for the metallo–dielectric cavity is shown in Figure 1b, where we use a surrounding air region of variable characteristic length, $d_{\text{air}}$. Figure 1c shows the $V_{\text{eff}}$ values of the five $V_{\text{eff}}$ expressions listed in Section 2 as a function of $d_{\text{air}}$, with the latter ranging from 795 nm to 3180 nm, or from about half of the upper photoluminescence (PL) boundary of InGaAsP to two times of it. For the metallo–dielectric cavity, among all five $V_{\text{eff}}$ expressions, $V_{\text{eff},1,2,3}$ expressions yield an identical result, and $V_{\text{eff},4,5}$ expressions show a slightly smaller value due to the surface and PML integral terms added to the norm. The maximum difference between $V_{\text{eff},1,2,3}$ and $V_{\text{eff},4,5}$ is only 1.12%, which agrees with our analysis in Section 2. The dependence of $V_{\text{eff}}$ on $d_{\text{air}}$ is seen to be negligible, and the small variation is most likely attributable to the different meshes that are generated upon changing $d_{\text{air}}$ and not related to any physical features of the modal profile.

3.2. Coaxial Resonator with Ag

A cross section of the Ag-cladded coaxial cavity is shown in Figure 2a, where $|E(r)|$ of the transverse electro-magnetic-like (TEM-like) mode is plotted. The cavity is enclosed by a spherical simulation space shown in Figure 2b. Despite the fact that the optical mode is fairly well confined to the active region of the cavity, there is notably more leakage into the air plug compared to the metallo–dielectric cavity. As a result, the electric field antinode is located in the air plug rather than the active region of the cavity. The quality factor of this plasmonic mode in the coaxial cavity is
on the order of 100, which is about an order of magnitude lower than the photonic mode in the metallo–dielectric cavity.

Figure 2. (a) Closeup of the TEM-like mode of the coaxial cavity with Ag as cladding material (lengths expressed in nm). (b) Side view of the entire spherical simulation space for the coaxial cavity. ($Q = 79.074$ at $2.0542e14$ Hz ($\lambda_0 = 1459.4$ nm)).

The evaluated effective modal volumes of the Ag-cladded coaxial cavity are shown in Figure 3, for various simulation conditions, which include different meshing finesse and simulation domain sizes. As the electric field maxima and electric field energy density maxima located in the air region and active region respectively, $V_{\text{eff},3}$ has the largest denominator among all five $V_{\text{eff}}$ expressions. Therefore, $V_{\text{eff},3}$ exhibits the smallest values. As $V_{\text{eff},2}$ takes the electric field energy density in its denominator, this $V_{\text{eff}}$ expression is less sensitive to the change of simulation domain size, and is the most stable one. Among the other three expressions, as the field quickly vanishes at the simulation boundary, $V_{\text{eff},1}, V_{\text{eff},4}$ and $V_{\text{eff},5}$ all show converging values with less than 30% variation ($V_{\text{eff},1} \approx 1.29 V_{\text{eff},4}$ and $1.27 V_{\text{eff},5}$) for all simulation conditions. From Figure 2a, it is apparent that the maximum electric field resides in the air region, which leads to a denominator for $V_{\text{eff},1}, V_{\text{eff},4}$ and $V_{\text{eff},5}$ that is significantly smaller than the denominators of both $V_{\text{eff},2}$ and $V_{\text{eff},3}$. Hence, the values of $V_{\text{eff},1}, V_{\text{eff},4}$ and $V_{\text{eff},5}$ are significantly greater than those of $V_{\text{eff},2}$ and $V_{\text{eff},3}$. Due to this same reason, $V_{\text{eff},1}, V_{\text{eff},4}$ and $V_{\text{eff},5}$ are more sensitive to the change of simulation domain size compared to $V_{\text{eff},2}$. Comparing Figures 3a and 3b, which present results for fine and normal meshing, respectively, we observe a rather negligible change in the evaluated expression of $V_{\text{eff},2}$. However, it is important to note that because $V_{\text{eff},1}, V_{\text{eff},3}$, $V_{\text{eff},4}$ and $V_{\text{eff},5}$ are normalized with respect to the maximum electric field density as in the case of $V_{\text{eff},2}$, if this maximum lies in the air domain, then the mesh size could play an important role. For example, this singularity of the field produced by the corners of the Ag core can be suppressed by reducing the mesh size [33]. Additionally, the accuracy of the simulation can be further improved by introducing the idea of subpixel smoothing of the isotropic dielectric function [34].
Figure 3. Effective modal volume of the coaxial cavity using Ag as metal for various simulation conditions, using (a) fine meshing and (b) normal meshing. $\lambda = 1590$ nm, which corresponds to the upper boundary of emission bandwidth of InGaAsP. Note that the traces for $V_{\text{eff},4}$ and $V_{\text{eff},5}$ are nearly identical.

3.3. Coaxial Resonator with AZO

A cross section of the AZO-cladded coaxial cavity is shown in Figure 4a, along with the simulation space in Figure 4b. It is evident that the mode is rather poorly confined to the active region with a substantial portion of modal energy escaping the cavity. Hence, this cavity functions more as an optical antenna with a quality factor on the order of 10, one and two orders of magnitude smaller than the coaxial cavity with Ag and the metallo-dielectric cavity, respectively.

Figure 4. (a) Closeup of the mode of the coaxial cavity with AZO (aluminum-doped zinc oxide) as cladding material (dimensions of all material regions are identical to coaxial cavity with Ag). (b) Side view of entire spherical simulation space. ($Q = 6.6884$ at $2.2991 \times 10^{14}$ Hz ($\lambda_0 = 1304.0$ nm).)

The evaluated effective modal volumes of the AZO–coaxial cavity are shown in Figure 5a, for various simulation conditions. These conditions include the spherical air domain of varying $d_{\text{air}}$ values. $V_{\text{eff},1}$, $V_{\text{eff},2}$, and $V_{\text{eff},3}$ yield diverging and identical results, increasing nonlinearly as $d_{\text{air}}$ increases from $0.5\lambda$ to $2.0\lambda$, thus these three $V_{\text{eff}}$ do not have a well-defined value. On the contrary, $V_{\text{eff},4}$ and $V_{\text{eff},5}$ show converged $V_{\text{eff}}$ values. The converged effective modal volume values are attributed to the surface integration term in Equation (10) and the PML integration term in Equation (14), which compensates the diverging volume integration term.
While AZO exhibits an attenuation coefficient one to two orders of magnitude smaller than that of Ag over the spectral range of emission of InGaAsP (see Figure 5b), the absolute value of the real part of the AZO permittivity is close to unity, which leads to more of the mode residing in AZO and thus leading to a spatially divergent field because of the impedance match with the surrounding air domains. Therefore, it becomes problematic to define the quasi-normal mode (QNM) norm with some integral of electromagnetic field over the entire space. In this sense, \( V_{\text{eff}},4 \) and \( V_{\text{eff}},5 \) provide a way for the normalization of QNM of low-Q cavities or plasmonic resonators, i.e., non-Hermitian systems.

4. Discussion

Based on the results, the type of cavity clearly affects the robustness of the various expressions of \( V_{\text{eff}} \) found in the literature. To quantify the stability of a \( V_{\text{eff}} \) expression, we use the maximum percentage difference, defined as:

\[
\Delta_{(#)} = \left( \max \left( \frac{V_{\text{eff},m}(#) - V_{\text{eff},n}(#)}{V_{\text{eff},m}(#)} \right) \right) \times 100\%
\]

where \( m \) and \( n \) refer to different simulation conditions. All the evaluation results are tabulated in Table 3 for fair comparison of the five effective modal volume expressions.

If the cavity supports a well-confined photonic mode, the electric field maximum resides in the active region and the five expressions yield nearly identical results if numerical error can be eliminated. This is confirmed with the metallo–dielectric cavity, where we observed that \( \Delta 1 = \Delta 2 = \Delta 3 \approx \Delta 4 \approx \Delta 5 < 0.21\% \) as the simulation domain size increases. This can be considered a negligible change.

For cavities supporting plasmonic modes, the proximity of the cavity resonance to the metal plasma frequency plays an essential role in determining the efficacy of the \( V_{\text{eff}} \) expressions. For the Ag–coaxial cavity under fine meshing, \( \Delta 2 < 2.02\% \), suggesting it is the most robust expression. However, for the AZO cavity, \( V_{\text{eff},1}, V_{\text{eff},2}, \) and \( V_{\text{eff},3} \) all diverge nearly at the same rate, while \( V_{\text{eff},4,5} \) converge but oscillate around certain values. Therefore, based on their robustness performance, for confined mode \( V_{\text{eff},2} \) is suggested; for leaky mode, \( V_{\text{eff},4,5} \) are suggested to obtain a more precise effective modal volume value. In addition, the choice of the correct effective modal volume formula should rely on a solid physical understanding of where the light–matter interaction of interest is happening.
In addition, notice that all five $V_{\text{eff}}$ formulae shown here only calculate the electric energy in the physical domain (including cavity and background material). However, for metallic cavities, especially at room temperature in the near-IR regime, the significant absorption loss of plasmonic or hybrid modes will result in unequal electric and magnetic energy in the cavity. For example, in the Ag–coaxial cavity, the electric energy is usually two to five times greater than the magnetic energy in the same material region. Therefore, calculating only the electric energy in metallic cavities should be understood as an approximation, and the $V_{\text{eff}}$ formulae should be modified for plasmonic modes if greater accuracy is desired [15,16,21].

5. Conclusions

We have identified five expressions in the literature commonly used for calculating the effective modal volume of resonant cavities. We evaluated and compared these expressions in the context of several canonical geometries supporting photonic and plasmonic modes for near-infrared nanoscale light sources. These included a metallo-dielectric cavity and coaxial cavities with Ag and AZO as cladding material. In the metallo-dielectric cavity, the various $V_{\text{eff}}$ expressions yield the same result and are robust to simulation domain changes because the electric field maximum resides in the active region. In the coaxial cavity, the $V_{\text{eff}}$ expressions yield results of varying stability due to the electric field and electrical energy density maxima residing in different regions. For low Q coaxial cavities, QNMs are no longer of finite energy, so standard QNM normalization methods based on energy consideration cannot be applied because of the spatially diverging field at large distance. Therefore, only $V_{\text{eff},4}$ and $V_{\text{eff},5}$ yield non-diverging results. Because of the relation of the effective modal volume to important quantities of theoretical and practical interest, such as the Purcell factor and spontaneous emission factor, our work conveys important results on the utility of the effective volume technique and its limitations.

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