



Designing structures that maximize spatially averaged surface-enhanced Raman spectra: erratum

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Abstract: This erratum corrects a misstatement regarding the absence of non-integrable singularities in 2d distributed Raman sensing applications and a formula [Eq. (9)] for one case of Raman enhancement. These changes do not impact the other results presented in the original manuscript [[Opt. Express](#) **31**, 4964 (2023)].

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1. Erratum

1.1. Non-integrable geometric singularities in 2d

In the vicinity of sharp geometric wedges, "hot-spots" in the electric field emerge. Sec. 2.4. *Corner singularities and hot spots* describes field singularities of the electric field \mathbf{E}_1 as a fractional power law in the distance r from the tip of a geometric singularity as described in [1]:

$$\mathbf{E}_1 \propto r^{t-1} \quad (1)$$

t can be solved via a transcendental equation depending on the angle ϕ and ε . The original manuscript [2] correctly states that the singularity is always integrable in 2d (but not 3d) for dielectrics ($\text{Re } \varepsilon > 0$). However, non-integrable singularities can be found for metals ($\text{Re } \varepsilon < 0$) such as silver at specific 2d angles. For example, a 35° silver 2d corner for $\lambda = 540\text{nm}$ ($\text{Re } \varepsilon = -12.4$) results in a non-integrable singularity with $t \approx 0.3$.

Nevertheless, these singularities are weak enough that they do not appear in freeform topology optimization of metals such as the ones in our paper, because the finite computational "mesh" resolution is enough to dampen/regularize the singularity. (We find that a sharp corner only arises from topology optimization if we build a high-resolution corner of the correct angle into the mesh *a priori*.) In manufacturable designs, corner singularities are prohibited by imposing lengthscale constraints [3]. Physical metals also exhibit nonlocal effects at few-nm lengthscales [4] that suppress corner singularities. As the original manuscript correctly notes, such regularizations are also necessary to suppress non-integrable corner singularities (even for dielectrics) in 3d.

1.2. Single-channel simplification: correction to Equation 9

In the case of an isotropic Raman-active molecular distribution, Eq. (8) simplifies to the following expression for the spatially averaged surface-enhancement:

$$\langle P \rangle_\alpha = \int |\alpha_0(\mathbf{x})|^2 |\mathbf{E}_1(\mathbf{x})^* \cdot \mathbf{E}'_2(\mathbf{x})|^2 d\Omega \quad (2)$$

This equation should replace Eq. (9) in the original manuscript, which incorrectly expressed the integrand as $|\mathbf{E}_1(\mathbf{x})|^2 |\mathbf{E}'_2(\mathbf{x})|^2$.

The numerical simulations in the original manuscript were correct, however, as they employed the correct expression above. Moreover, the further simplification to $|\mathbf{E}_1(\mathbf{x})|^4$ (for the $\mathbf{E}_1 = \mathbf{E}'_2$ case where the pump and emission frequencies and angles coincide) remains correct. Therefore, the results and conclusions of the paper are unaffected.

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