

Spectral-crystal efficiency mapping: An analytical tool for visualizing the parametric conversion potential of broadband sources

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Quasi-phase-matching in $\chi^{(2)}$ media underpins many nonlinear conversion techniques, yet conventional sinc-squared gain models assume monochromatic pumps and wavelength-independent efficiency, limiting their accuracy for broadband sources. We introduce spectral-crystal efficiency mapping (SCEM), an analytical framework that combines input spectra with the nonlinear properties of a crystal to evaluate conversion potential. SCEM incorporates pump spectral profiles, higher-order interactions, and cascaded processes, providing an upper bound on efficiency that complements more computationally demanding numerical models. The resulting maps agree with experiment and simulation, while offering experimentalists an intuitive tool for assessing nonlinear gain media and guiding optimization of broadband frequency-conversion systems.

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I. INTRODUCTION

Quasi-phase-matching (QPM) is a pivotal technique in nonlinear optics, enabling efficient frequency-conversion processes by periodically modulating the nonlinear coefficient of a material. The conventional approach to calculating gain in a QPM medium is via a sinc-squared gain function, which stems from solving a set of three coupled wave equations describing the efficiency of nonlinear interactions as a function of phase mismatch [1]. This method, while foundational, has notable limitations that hinder its applicability in more complex scenarios.

The sinc-squared gain function assumes a monochromatic pump spectrum, and relies on the user's due diligence in adapting results to the spectral profile of their pump laser. The sinc-squared equation,

$$\text{Gain} \propto \left| \frac{\sin\left(\frac{m\Delta kL}{2}\right)}{\frac{m\Delta kL}{2}} \right|^2, \quad (1)$$

where m is the QPM order; Δk is the wave-number mismatch; and L is the interaction length, predicts gain for idealized pump pulses (single k value) in perfectly periodic gratings with a 50:50 duty cycle. This approach,

however, fails to account for the frequency-dependent nonlinearity of the crystal [1] or the presence of complex spectral shapes in real pump pulses. These deficiencies limit the conventional method's accuracy and applicability, particularly in advanced applications employing broad bandwidth pulses and those requiring precise control over frequency-conversion processes. Improved gain-calculation techniques that can incorporate these complexities are essential for rapid, cost-efficient development of next-generation QPM devices, enabling their use in a broader range of scientific and industrial applications. The fact that the sinc-squared equation is still regularly used in the design of ultrafast systems [2–7], despite its monochromatic form, highlights the need for a tool that can more appropriately fill the role.

Here, we demonstrate a method for more complete analysis of the potential parametric conversion efficiency resulting from the combination of one or more input spectra and a nonlinear crystal, with results which can be easily interpreted by means of a spectral-crystal efficiency map (SCEM). Beginning from first principles, we introduce an idealized SCEM for spontaneous parametric down-conversion (SPDC) from a pump pulse with a top-hat spectral profile, before incorporating the power-conversion efficiency of the nonlinear process and measured spectral intensity profiles. Expanding to higher-order and cascaded interactions, we show that a baseline crystal efficiency map need only be calculated once for a given crystal, and subsequently filtered with a pump spectral envelope to determine the full spectral-crystal efficiency map. This analytical approach agrees strongly with more

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computationally demanding numerical simulations, and is better suited for providing insight into the feasibility of accessing different spectral regions, removed from the limits imposed by specific temporal dynamics. Finally, we demonstrate the efficacy of our approach by comparing SCEMs of several nonlinear crystals against published experimental results employing synchronously pumped optical parametric oscillators (OPOs).

The SCEM methodology bridges the gap between traditional quasi-phase-matching calculations and the complexities of real-world frequency conversion. Starting from an idealized model and incorporating realistic parameters such as pump spectral profiles and cascaded interactions, SCEM provides an efficient framework for evaluating nonlinear gain media. Like the familiar sinc-squared approach, SCEM is not intended to replace numerical simulations [8–13] but instead offers experimentalists an intuitive, phase-agnostic view of the accessible spectral space. Producing equivalent maps with full-field solvers requires extensive parameter sweeps across temporal and spectral dimensions, making them computationally demanding and impractical for rapid exploration. In contrast, SCEM delivers the complete conversion landscape in a few analytical steps, guiding optimization efforts and helping avoid time spent pursuing unachievable outputs.

II. THEORY

A. Parametric gain equation

The derivation of the sinc-squared gain equation is covered in detail in other literature, nevertheless, a summary is given here for clarity and commentary. We start from the coupled wave equations derived in Sec. 2.2 of Boyd [1]. Working under the slowly varying envelope approximation, for the signal amplitude (A_s) resulting from difference frequency generation (DFG) between monochromatic, constant amplitude pump and idler (A_p, A_i), we have

$$\frac{dA_s}{dz} = \frac{2id_{\text{eff}}\omega_s}{n_s c} A_p A_i^* e^{-i\Delta k z}, \quad (2)$$

where A_s is a slowly varying function of distance z ; $\omega_p > \omega_s \geq \omega_i$ are angular frequencies; n_s is the refractive index of the nonlinear medium at ω_s ; and d_{eff} is the effective nonlinear coefficient.

Integrating over z from 0 to crystal length L and converting amplitudes into intensities (I_p, I_s, I_i) results in

$$I_s = I_p I_i L^2 \frac{2d_{\text{eff}}^2 \omega_s^2}{n_p n_s n_i \varepsilon_0 c^3} \text{sinc}^2(\Delta k L / 2), \quad (3)$$

where ε_0 is the vacuum permittivity. A more complete derivation of Eq. (3) is provided in Appendix A.

The resultant signal intensity I_s is dominated by the sinc-squared phase-mismatch term, and is weighted by

two prefactors, which are often ignored: an extrinsic term arising from the length of the nonlinear crystal and the spectral intensity profiles of the pump and idler waves, and a power-conversion efficiency term intrinsic to the nonlinear process and the crystal material. These prefactors will be discussed in Sec. II C.

Equation (3) cannot be applied directly to broadband radiation because it does not capture the phase relationship between different spectral components within a single pump pulse. The spectral phase profile determines which phase-matched processes are preferentially enhanced and the relative strength of those interactions. However, since Eq. (3) implicitly assumes optimal initial phase conditions for each interacting field, it still accounts for all processes that are permitted by phase matching, even in the broadband case. Put differently, spectral components that cannot satisfy phase-matching conditions remain inaccessible regardless of the chosen phase profile. More generally, there is no closed-form analytical solution for phase matching in broadband nonlinear evolution: the coupled dynamics of arbitrary spectral envelopes and cascaded interactions can only be resolved numerically [1]. SCEM therefore exploits the spectral-only form of Eq. (3) to provide an upper bound on the potential gain in broadband systems, while leaving experimentalists free to tune the temporal characteristics of the physical system to select and optimize specific outputs.

B. Creating a simple SCEM

For a periodically poled crystal with a given dispersion relation and length, the parametric gain equation highlights the possible wavelengths obtainable when combining a monochromatic pump pulse with an idealized grating. For a crystal with multiple gratings, a common approach is to calculate the relative gain at equidistant sample periods, Λ_G , across the operational range. To demonstrate the SCEM concept we consider SPDC in a 5-mm-long fan-out PPLN crystal ($d_{\text{eff}} = 2d_{33}/\pi = 17 \text{ pmV}^{-1}$ [14]), with grating periods of 27.5–32.5 μm , at a temperature of 34 °C pumped at $\lambda_p = 1.03 \mu\text{m}$. The wave-number mismatch between one combination of pump, signal, and idler, at a fixed grating period Λ_G is

$$\Delta k_Q = 2\pi \left(\left| \frac{n(\omega_p)}{\lambda_p} - \frac{n(\omega_s)}{\lambda_s} - \frac{n(\omega_i)}{\lambda_i} \right| - \frac{m}{\Lambda_G} \right), \quad (4)$$

where the signal wavelength (frequency) is a function of the two input components, and with QPM order, m , accounting for phase matching over multiple domains. Our initial pump wavelength is single valued, resulting in a two-dimensional (2D) parameter space, $(\lambda_i, \Lambda) \in (\lambda_p, 6 \mu\text{m}) \times [27.5, 31.5] \mu\text{m}$, so for coarsely sampled Λ , each gain profile is represented by a simple curve as shown in Fig. 1(a).

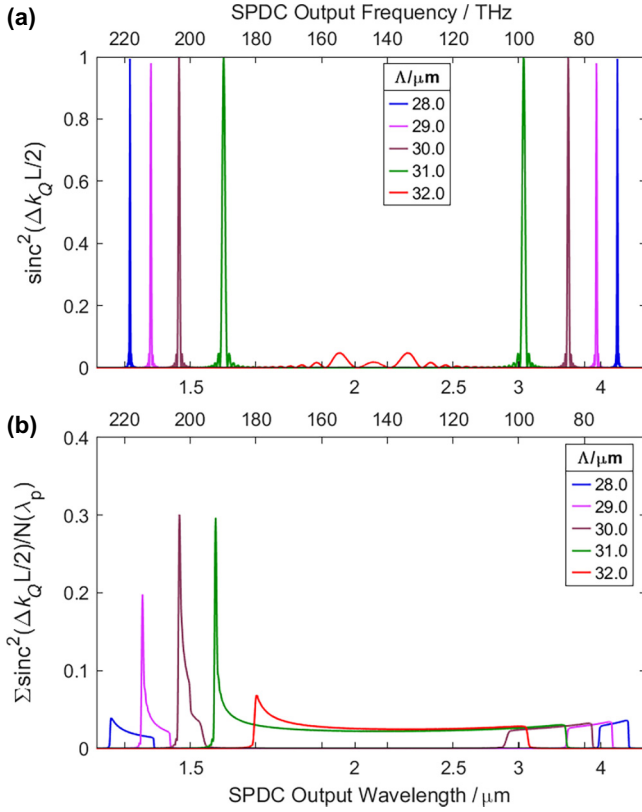


FIG. 1. (a) SPDC phase-mismatch profiles in a coarsely sampled fan-out PPLN crystal using a monochromatic pump wavelength. Each curve displays the characteristic sinc-squared profile. (b) SPDC phase-mismatch profiles in the same crystal using a top-hat pump spectrum.

Significantly increasing the grating sampling resolution allows us to plot an *efficiency map* for this combination of monochromatic pump pulse and fan-out PPLN crystal, as shown in Fig. 2(a). This efficiency map is unweighted and normalized since we currently ignore the prefactors in Eq. (3).

Repeating the sinc-squared calculation for a number of different pump wavelengths within some linewidth, $\Delta\lambda_p$, extends the parameter space for the initial sample grating plots into 3D, $(\lambda_p, \lambda_i, \Lambda) \in [\Delta\lambda_p] \times (\min(\Delta\lambda_p), 6 \mu\text{m}) \times [27.5, 31.5] \mu\text{m}$, with a representative plot shown in Fig. 3. For each discrete Λ_G , the familiar, m th-order QPM curve from the conventional family, $Q_\Lambda : \Omega_p \times \Omega_i \rightarrow [0, 1]$, $(\omega_p, \omega_i) \mapsto Q(\omega_p, \omega_i, \Lambda_G)$ is given by

$$Q_\Lambda(\omega_p, \omega_i) = \text{sinc}^2(\Delta k_Q(\omega_p, \omega_i)L/2)/m^2. \quad (5)$$

At this point, the curves in Fig. 3 represent nothing more than variations of Fig. 1(a) as a function of wavelength, with each λ_p still representing a single, independent, monochromatic pulse. Summing over the pump wavelengths (dividing by the number of components for normalization) allows us to create the actual analog to Fig.

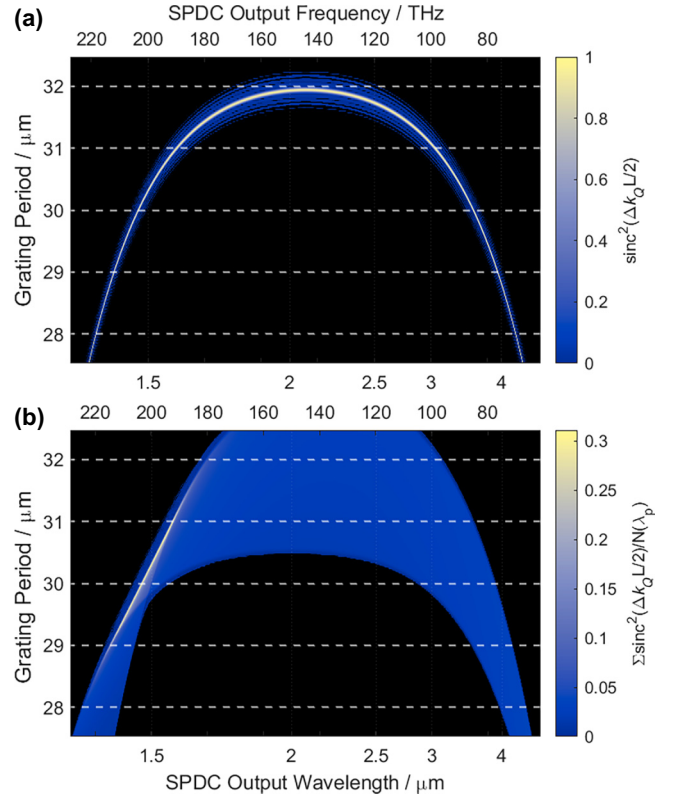


FIG. 2. (a) Two-dimensional efficiency map of a continuously sampled fan-out PPLN crystal and monochromatic pump. Dashed lines correspond to the coarsely sampled grating periods shown in Fig. 1(a). (b) Idealized SCEM of a continuously sampled fan-out crystal and a top-hat pump spectrum. The 2D gain profile indicates high gain concentration around $\omega_s = 1.48 \mu\text{m}$ and $\Lambda = 30 \mu\text{m}$.

1(a), this time for an idealized top-hat pump pulse with nonzero linewidth [Fig. 1(b)].

Here we can see that the gain profile resulting from multiple different pump components no longer resembles the constituent sinc-squared functions; of note, the gain profile is no longer consistent across the DFG wavelength range. Returning to a pseudocontinuous sampling of Λ results in the simplest true (unweighted and highly idealized) SCEM [Fig. 2(b)].

Even this relatively simple SCEM gives a powerful indication of how the gradient of the conventional QPM curves impacts the available gain concentration for different DFG wavelengths. For the SPDC system described here it follows that there should be a region of high gain concentration around $\omega_s = 1.48 \mu\text{m}$ and $\Lambda = 30 \mu\text{m}$, corresponding to where the QPM curves are most vertical across the pump linewidth.

C. Incorporating prefactors

Two key pieces of information are lost by ignoring the prefactors in the conventional approach. The first is

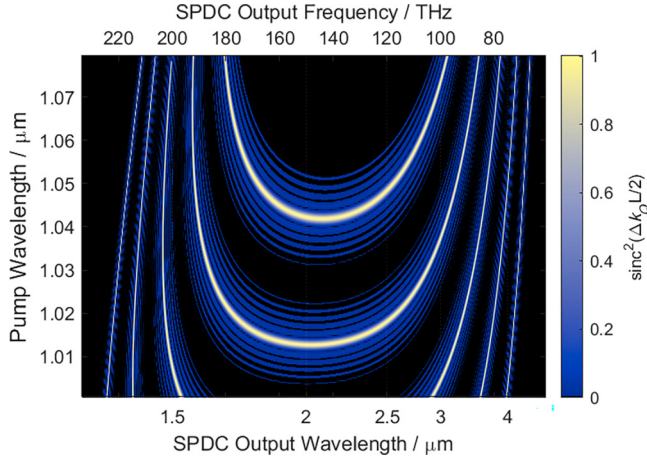


FIG. 3. Conventional, sinc^2 QPM curves for a coarsely sampled fan-out PPLN crystal ($L = 5$ mm, $T = 30^\circ\text{C}$) at multiple, discrete, monochromatic pump wavelengths. Sampled grating periods match those shown in Fig. 1(a), with the leftmost curve corresponding to $\Lambda = 28$ μm .

the power-conversion efficiency of the nonlinear process intrinsic to a given crystal material

$$P_\eta(\omega_p, \omega_i) = \frac{2d_{\text{eff}}^2 \omega_s^2(\omega_p, \omega_i)}{n_p n_s n_i \varepsilon_0 c^3}, \quad (6)$$

where P_η has units of W^{-1} . We plot P_η as a function of two inputs (rather than an input and the output as seen thus far) since each output wavelength can correspond to a range of power-conversion efficiencies, depending on the constituent inputs. An example power-conversion efficiency plot for DFG processes in PPLN is shown in Fig. 4.

The second missing piece of information is the combined effect of the crystal length and the spectral intensity

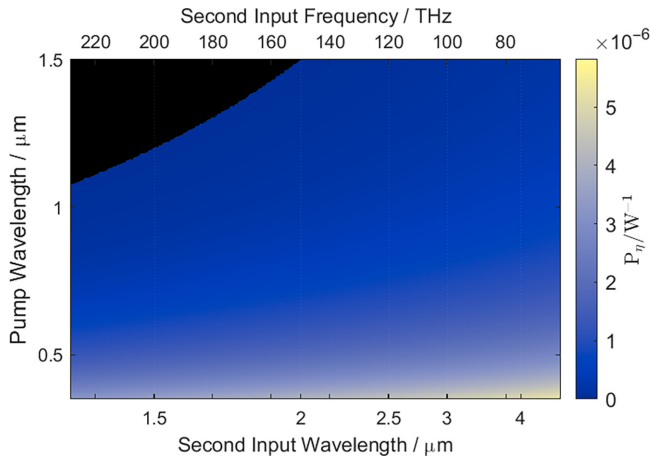


FIG. 4. Power-conversion efficiency for DFG processes in PPLN as a function of the two inputs. The black region indicates interactions forbidden by energy conservation.

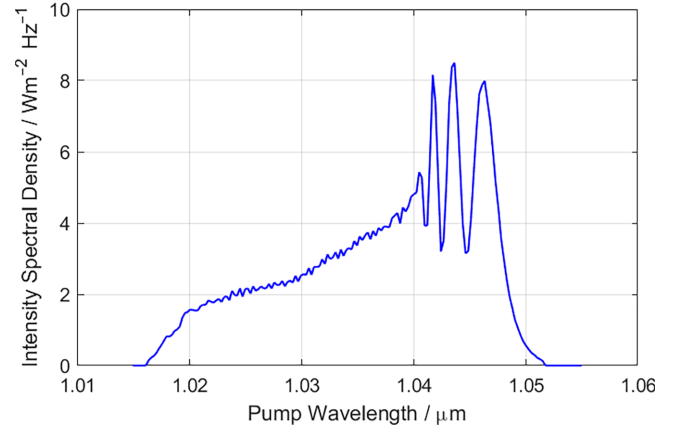


FIG. 5. Experimental pump spectrum, recorded from an amplified Yb: fiber laser [16].

profiles of the input pulses. In a hypothetical setup, one might wish to use a normalized pump pulse shape, scaled such that $\Sigma I_p(\omega) = 1$. In this scenario the output can be interpreted as a maximum potential gain relative to an undepletable pump pulse, e.g., idealized OPO.

When considering real pulses of finite bandwidth, with arbitrary spectral profile, we instead work with discretized intensity spectral density (ISD), denoted $\tilde{I}(\omega)$ for convenience, and defined such that $\sum_{\omega \in \Omega} \tilde{I}_p(\omega) \Delta \nu = I_p$, for any choice of spectral window resolution, $\Delta \nu$. Note that the validity of the 2D frequency sample space is no longer defined by the pulse bandwidths, so Eqs. (3), (5), and (6) combine to give

$$\tilde{I}_s(\omega_1, \omega_2) = \tilde{I}_p(\omega_1) \tilde{I}_i(\omega_2) L^2 P_\eta(\omega_1, \omega_2) Q_\Lambda(\omega_1, \omega_2), \quad (7)$$

for arbitrarily chosen $(\omega_1, \omega_2) \in \Omega^2$.

In this form, two real input spectra ($\tilde{I}_p, \tilde{I}_i$) can be used to calculate the maximum potential ISD out, assuming negligible depletion of either input pulse. In cases where I_i cannot be determined independently (e.g., SPDC, OPO), we rely on experimental and/or simulated examples to provide a suitable order of magnitude, and treat $\tilde{I}_i$ as a uniform scale factor representing the system's ability to seed from background field states. In our example system $I_p \approx 2 \times 10^{13} \text{ Wm}^{-2}$ with $\tilde{I}_p$ shown in Fig. 5, and we let $\tilde{I}_i(\omega) = 0.03 \text{ Wm}^{-2} \text{ Hz}^{-1} \forall \omega \in \Omega$, in accordance with numerical simulation [10,15].

More realistic predictions can be made for single-pass systems by accounting for the maximum power available for a particular frequency conversion process. To do this, when scaling the QPM gain array, the combined ISD of the input pulses act as an upper bound (see Appendix B 1).

Combining the input intensity scaling and conversion efficiency gives the weighted prefactors for a combination of realistic pump pulse and a particular $\chi^{(2)}$ process (Fig. 6). We now have all the ingredients needed to create a

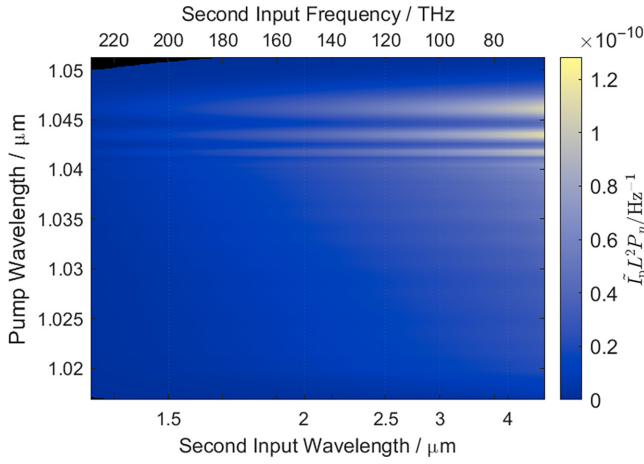


FIG. 6. Weighted SCEM prefactors combining intrinsic PPLN DFG conversion efficiency with our choice of crystal length and pump-intensity spectral density.

much more realistic SCEM for the SPDC process (Fig. 7). Comparing this result with Fig. 2 shows how much predictive power is offered by proper application of this SCEM technique. It is clear that optical parametric generation (OPG) based on this combination of pump pulse and nonlinear crystal should not be expected to exhibit consistently strong, narrowband gain across its operational range, and steps can be taken to ensure the desired performance is available around different wavelengths of interest.

III. FULL SCEM WITH HIGHER-ORDER AND CASCADED NONLINEAR INTERACTIONS

A. Crystal-only efficiency maps

The baseline sinc-squared equation can only account for a single nonlinear process at a time, but the same principle

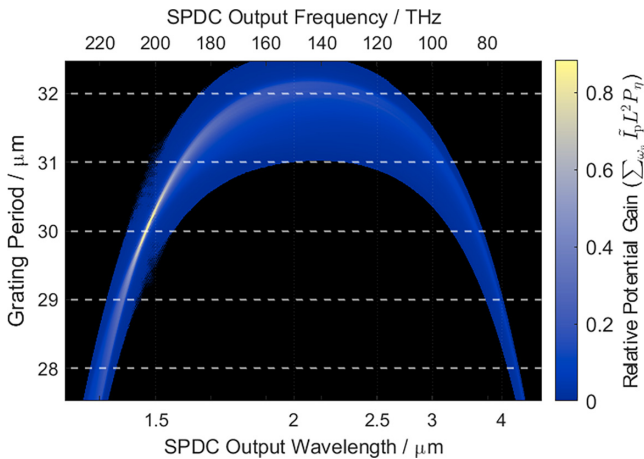


FIG. 7. Pump weighted SPDC spectral-crystal efficiency map indicating potential frequency conversion relative to the secondary input.

can be applied in different regimes, such as sum-frequency generation (SFG), to help build up an even more complete picture of possible spectral-crystal interactions. The SCEM for one process can also be used as a weighting map for subsequent cascaded processes.

The most elegant way to build up a full analytical SCEM is to begin by considering the whole possible phase-matching space for the crystal alone: the crystal efficiency map (Fig. 8).

The 2D frequency parameter space is chosen such that $\omega_1, \omega_2 \in \Omega$ are symmetrically sampled, producing a square phase space. Maintaining a common domain is crucial for modeling cascaded processes, as we discuss in later sections. These crystal efficiency maps are generated separately for SFG and DFG phase spaces, and include odd-valued higher-order phase-matching terms. For DFG $m = [1, 3]$ and for SFG $m = [1, 3, 5]$, since the fifth-order SFG interactions are the most relevant within the range of our sample grating periods (any range of values can be used, but we avoid irrelevant higher-order QPM to reduce computation time).

Each kind of frequency generation process has its own inherent conversion efficiency, which can be used to weight the basic crystal efficiency map, but no intensity scaling is applied at this point. This is equivalent to assuming two square-wave input pulses with nondepletable, uniform ISD of $1 \text{ Wm}^{-2} \text{ Hz}^{-1} \forall \omega \in \Omega$.

The addition of SFG processes highlights a key complexity in correctly representing the SCEM for anything beyond the idealized SPDC example given in the previous section. It is simple enough to plot wave-number mismatch (Δk_Q) as a function of input wavelengths, but this is significantly less helpful than illustrating Δk_Q in terms of the resultant, output wavelength. When plotting conventional QPM curves, one simply uses the output wavelength array to provide x -axis values (one can also leverage the symmetry of DFG to allow direct swapping of the signal and idler axes), but this array will be different for each process. Combining results into a single map requires careful transformation onto a single common basis (see Appendix B 2).

Having calculated the crystal-only efficiency map for the full set of gratings and over the entire relevant spectral range (i.e., the crystal transparency window), no further phase-matching calculations need to be performed. Instead, we can use the pump pulse envelope as a spectral filter to pick out the initial frequency generation, add the resulting SCEM to the filter, and repeat the process to account for other, often cascaded, processes. We generalize the previous ISD scaling expression to a variable spectral filter, which incorporates the crystal length, such that

$$S_\Lambda(\omega_1, \omega_2) = \tilde{I}_1(\omega_1) \tilde{I}_2(\omega_2) L^2 \quad (8)$$

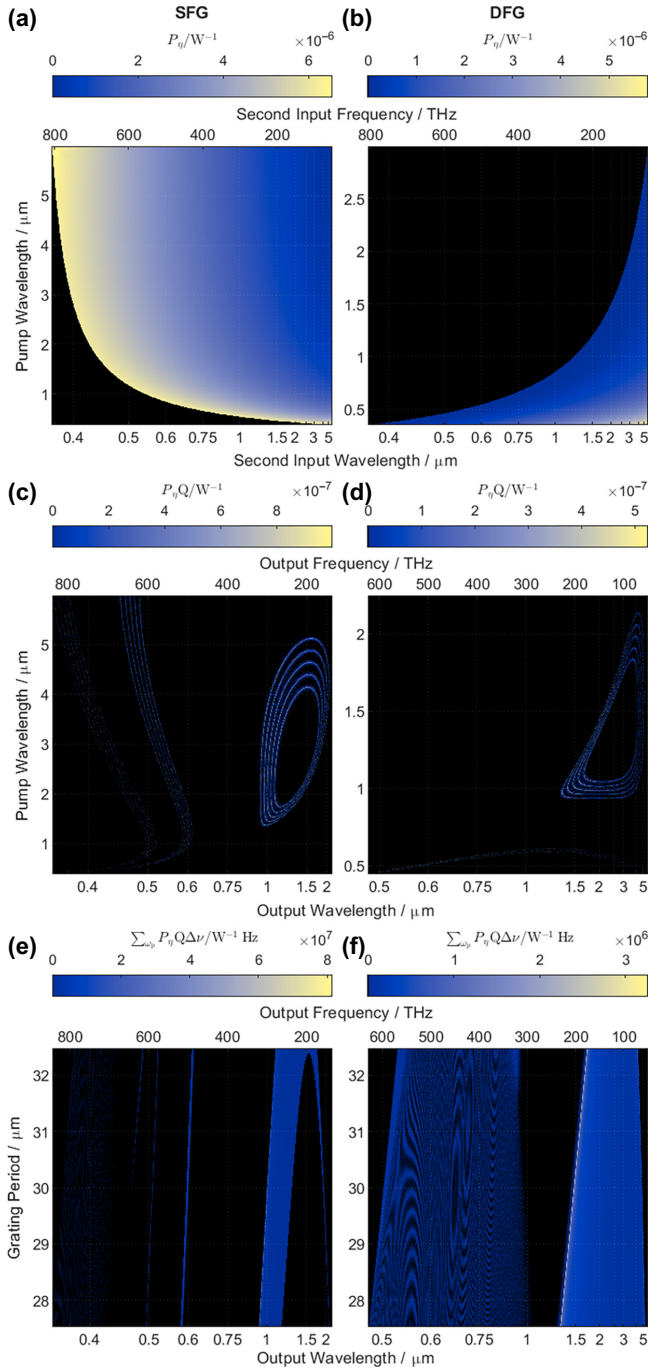


FIG. 8. PPLN conversion efficiency for (a) SFG and (b) DFG processes. Sample grating QPM curves from $\Lambda = [27.5 - 32.5] \mu\text{m}$ for (c) SFG, (d) DFG. Crystal-only efficiency maps for (e) SFG and (f) DFG.

resulting in a broadly applicable efficiency formula, which can be expressed in the untransformed, 3D input space simply as

$$\tilde{I}_3(\omega_1, \omega_2, \Lambda) = \sum_{\chi} SP_{\eta} Q \quad (9)$$

where $\sum_{\chi}$ indicates the sum over all relevant nonlinear processes. This allows us to add multiple layers of complexity to the map at reduced cost, since the QPM calculations are, by far, the most computationally expensive part of the procedure. In fact, the baseline crystal efficiency maps need only be calculated once for a given crystal, and they can then be stored for use with any future pulse source.

B. Pump SHG and SPDC

The first field component that develops during propagation through the PPLN crystal should be due to second-harmonic generation (SHG) from the pump. First-order phase matching for pump SHG occurs at much smaller grating periods, but is evident even at longer grating periods due to a combination of higher-order QPM and last coherence length effects in real-world crystals. Thanks to the incorporation of SFG up to fifth order in the crystal-only efficiency map, this pump SHG appears as expected after applying the pump filter to both input dimensions: $S_{1,2} = \tilde{I}_p \tilde{I}_p^T$ [Fig. 9(a)]. This 2D filtering is intrinsic to all SFG efficiency maps to prevent artificial “spontaneous up-conversion.”

For initial DFG, the pump filter is applied in one input dimension as before, with the second input scaled to account for gradual evolution of an idler field via parametric fluorescence [Fig. 9(d)]. The SPDC plot shown in Fig. 7 is reproduced in the resulting SCEM [Fig. 9(f)], demonstrating the consistency between this spectral filtering approach and direct calculation.

C. Cascaded processes

With SCEMs now calculated for SHG and SPDC interactions, the power of the sequential filtering approach quickly becomes apparent. Each grating period “slice” in the SCEM corresponds to a potential output spectrum, expressed in the same units as the initial pump profile, and defined on a common basis. Cascaded processes can be illustrated individually by utilizing the appropriate SCEM as a spectral filter, whilst the linearity of the operation also allows for multiple simultaneous processes through addition of each subsequent SCEM to a cumulative filter.

For example, the SPDC SCEM in Fig. 9(f) can directly be extended by accounting for the potential cascaded DFG between signal and idler waves. The cascaded spectral filter function is given by

$$S_{1,2} = (\tilde{I}_p + \tilde{I}_{\text{SPDC}})(\tilde{I}_p + \tilde{I}_{\text{SPDC}})^T \quad (10)$$

where $\tilde{I}_{\text{SPDC}}(\omega_1, \omega_2, \Lambda)$ is the full SPDC ISD map. As before, we plot the filtered conversion efficiency and resulting QPM curves for this process at equidistant sample grating periods, with the cascaded process acting as a $\chi_{\text{DFG}}^{(3)}$ effect, implicitly dependent on the pump frequency

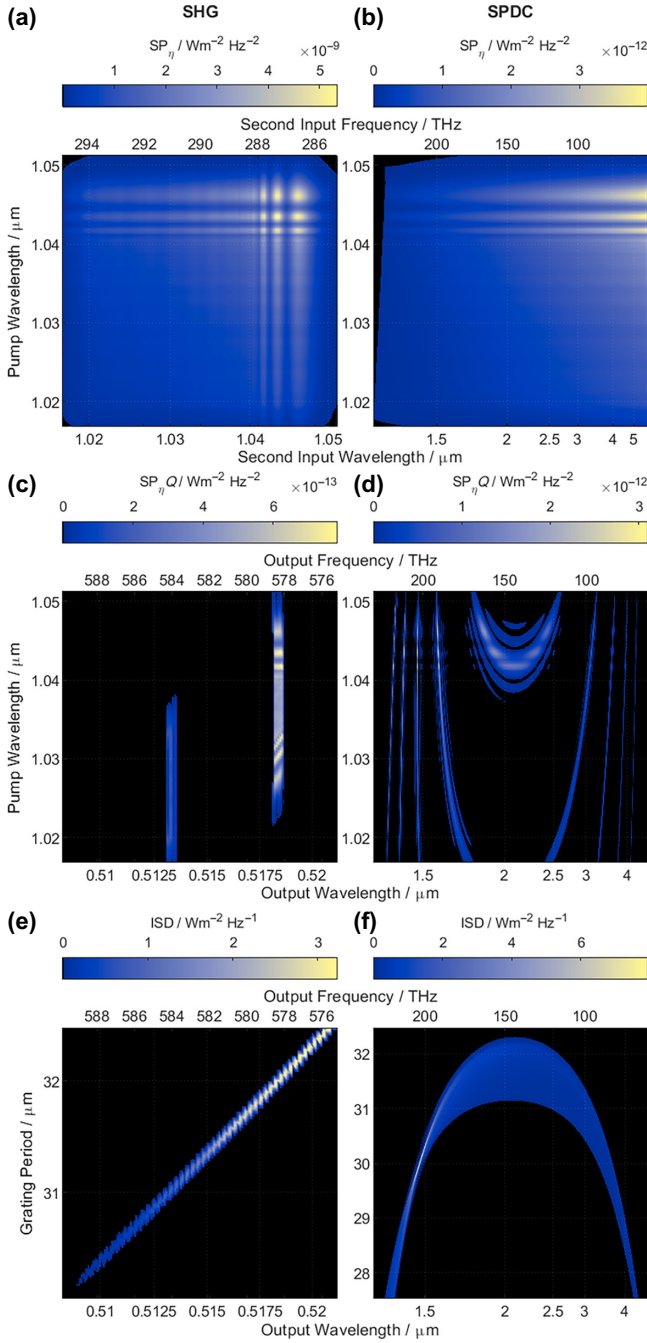


FIG. 9. Pump weighted conversion efficiency for (a) pump SHG, (b) SPDC. Sample grating QPM curves from $\Lambda = [27.5 - 32.5]$ μm for (c) pump SHG, (d) SPDC. SCEM for (e) pump SHG and (f) SPDC.

(Fig. 10). The cascaded filters and resulting SCEMs are shown individually for clarity, but a composite filter [e.g., the sum of Figs. 9(b) and 10(a)] would produce the combined SCEM directly.

All of this detail ultimately results in a single combined SCEM, which gives experimentalists an overview of a system's accessible spectrum, condensed into one image [Fig. 11(a)].

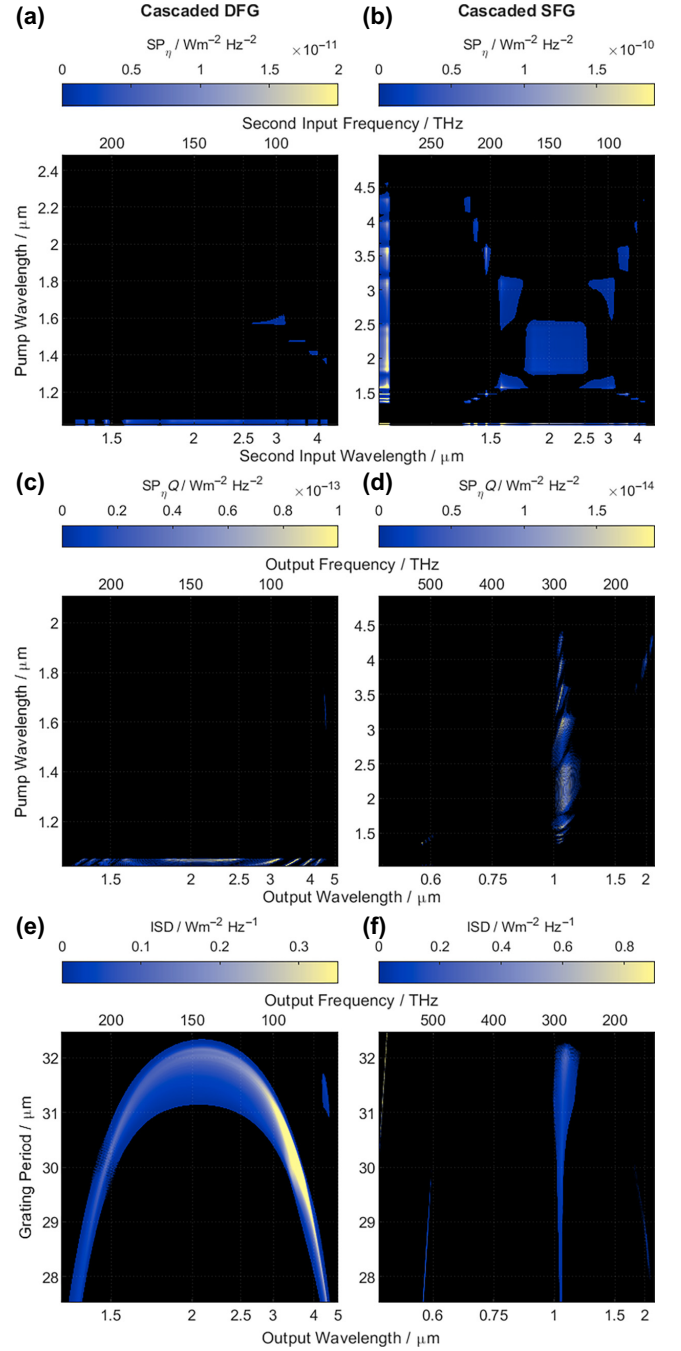


FIG. 10. Cascaded conversion efficiency weighted by initial SPDC for (a) DFG, (b) SFG. Sample grating QPM curves from $\Lambda = [27.5 - 32.5]$ μm for (c) DFG, (d) SFG. Additional SCEM for cascaded (e) DFG and (f) SFG.

IV. VERIFICATION AND FURTHER EXAMPLES

A. Comparison with simulation

The final SCEM in the previous section shows phenomenal agreement with numerical modeling of OPG [Fig. 11(b)] performed in the optical simulation software OptiFax [10,15], clearly showing the expected spectral

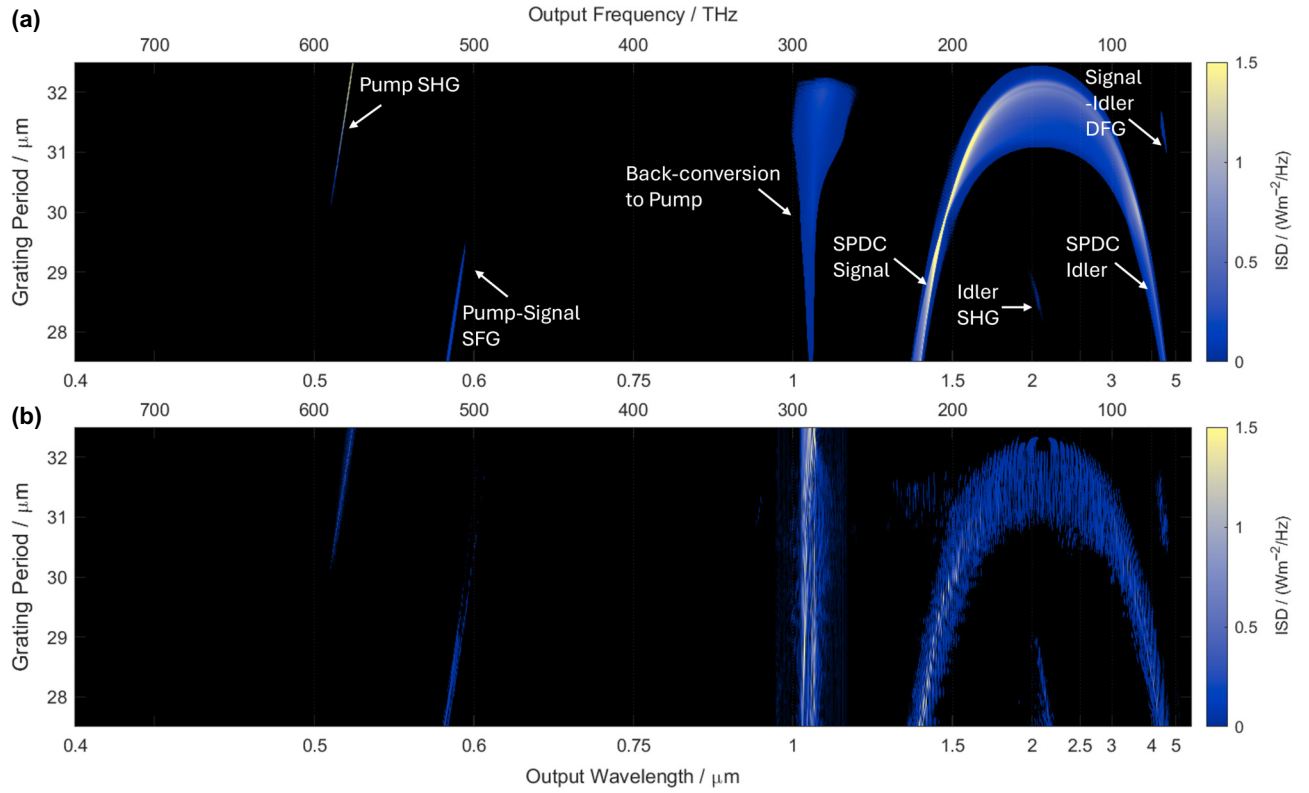


FIG. 11. (a) Combined analytical SCEM for a 3.76-W, 100-MHz, amplified Yb: fiber laser and 5-mm-long PPLN crystal. (b) Simulated single-pass output from NEE numerical simulation displayed in SCEM format for comparison. The key features indicated in the analytical SCEM are replicated here.

output across the entire parameter space in a single plot. These numerical simulations leverage the nonlinear envelope equation (NEE) and incorporate temporal dynamics, which preferentially select for particular wavelengths, but they therefore require lengthy parameter sweeps in order to identify all phase-matching possibilities. Conversely, by ignoring temporal dynamics, SCEM provides the full possibility space in a few analytical steps. As such, one-to-one correspondence between SCEM and the NEE is not expected, but we do expect each constrained NEE simulation to give a subset of the full SCEM. This makes SCEM an invaluable tool to be used in tandem with numerical modeling, offering a guide to a system's potential spectral output under the right conditions.

B. Periodically poled potassium titanyl phosphate (PPKTP)

Once implemented, the SCEM algorithm can easily be applied to a range of different systems. We utilize custom data structures implemented in OptiFax to quickly switch between optical sources, changing $\tilde{I}_p$; and to import other nonlinear crystals, changing refractive index, n_r ; material temperature, T ; and d_{eff} .

For example, PPKTP may be used when one wishes to leverage the wide gain bandwidth for broadband applications such as frequency combs for astronomical spectrograph calibration [17]. As shown in Fig. 2, the conventional QPM approach generally predicts constant gain across the full phase-matched region, which can be particularly problematic when evaluating the potential broadband response. In contrast, the SCEM shown in Fig. 12 for a 5-mm-long PPKTP crystal ($d_{\text{eff}} = 2d_{33}/\pi = 10 \text{ pmV}^{-1}$, $T = 100^\circ\text{C}$ [18,19]) pumped by the 1.16-W, 333-MHz, Ti:sapphire laser reported in Ref. [20], demonstrates significant variation in efficiency across the SPDC band. This SCEM also shows how the broad gain bandwidth of PPKTP can lead to greater complexity in the output of the cascaded nonlinear processes, resulting in yet more information, which is absent from the conventional sinc^2 QPM curves. Note that for this system we need to increase the maximum value of m for higher-order SFG processes (up to $m = 7$ from $m = 5$ in the previous section) in order to properly account for pump SHG. This parameter can be tuned for different systems by increasing the maximum value of m until the final SCEM results are unaffected.

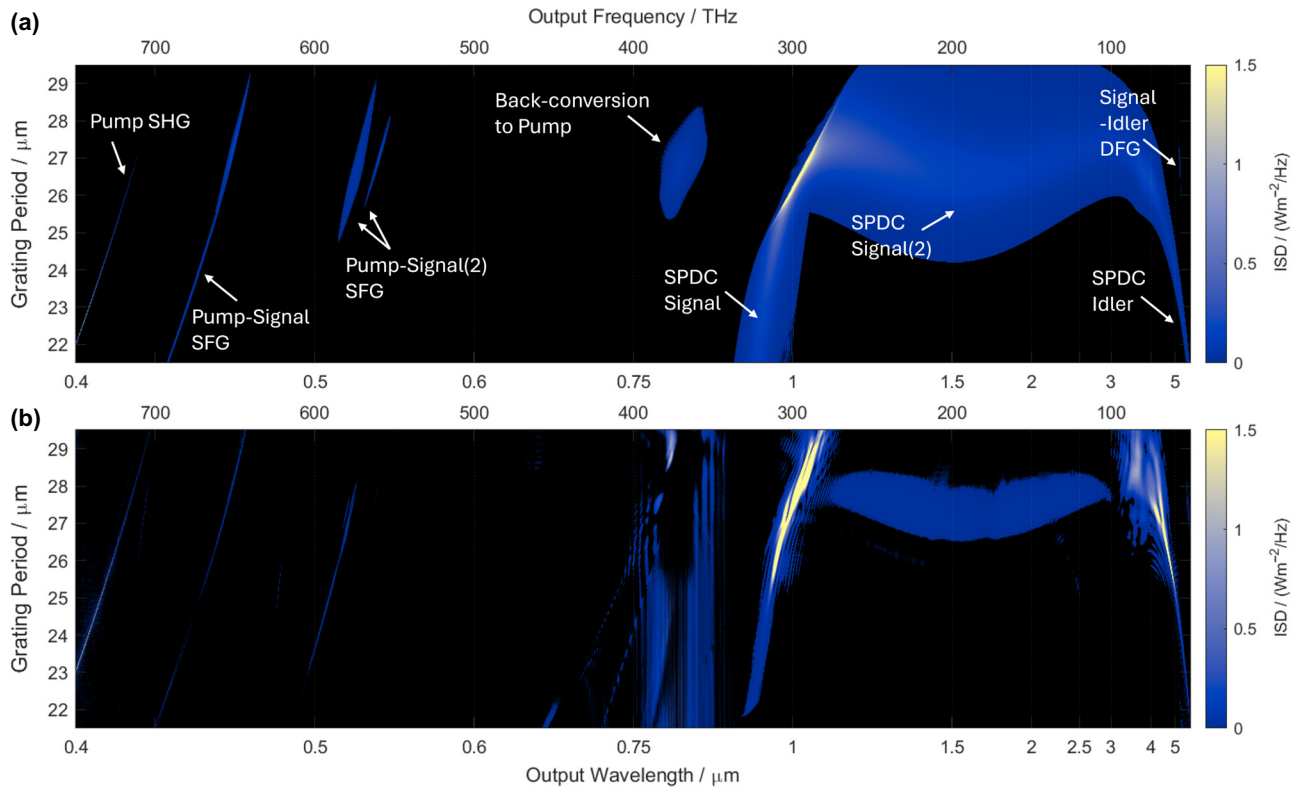


FIG. 12. (a) Full SCEM for 5-mm-long PPKTP crystal and 1.16-W, 333-MHz, Ti:sapphire laser. The build up of the composite filter from the individual nonlinear processes can be seen in Appendix C. (b) Simulated single-pass output from NEE numerical simulation displayed in SCEM format for comparison. The lack of broadband response for $\Lambda_G > \sim 28 \mu\text{m}$ demonstrates the significance of accounting for variation in QPM efficiency, as pump power is monopolized by the signal components shown with peak gain concentration in the plot above.

C. Tandem optical parametric oscillator

So far, we have used crystals with fan-out designs to vary the grating period across the aperture, with Λ_G remaining constant along the entire axis of propagation. However, the ability to use one SCEM as the input spectral filter when generating a second SCEM has applications beyond the mapping of cascaded processes for fixed poling periods. In cascaded grating OPO devices, a single crystal can be employed, which contains multiple different gratings in series [21]. These subsections can then each be optimized for a different conversion process, allowing for enhanced SHG, SFG or DFG outputs. Equivalently, a full SCEM can be generated for one subsection of a crystal and used as the initial spectral filter for the next, facilitating multiple full passes of the algorithm, where each nonlinear process is repeated for each subsection.

One example of a cascaded grating OPO is the idler-resonant tandem system reported in Ref. [22], in which the OPO contained a 2.6-mm-long PPLN crystal formed from two sections of 1.0- and 1.6-mm length, which had different grating periods, with seven grating pairs across the crystal height. An initial signal and resonant idler were generated in the first section with the signal acting as a

pump in the secondary grating, further transferring power to the resonant idler and generating a second idler at longer wavelengths, denoted in Ref. [22] as idler(2). The experimental setup and the crystal design are shown in Fig. 13(d). Tandem operation was realized when simultaneous phase matching was achieved in both sections of the crystal. Here we further demonstrate the capabilities of SCEM by analyzing this system, demonstrating the ability to predict and explain previously unexpected behavior.

The authors reported that it was not possible to experimentally study the nontandem behavior of the first grating due to the monolithic nature of the crystal. Figure 13(a) shows the SCEM for the first section in isolation, showing high conversion efficiency in two distinct signal bands centred around 1.08 and 1.27 μm in grating G . The corresponding idler bands are shown, centred around 3.87 and 2.49 μm , respectively. The longer idler region was observed in Fig. 6 of Ref. [22] and was attributed by the authors to single-pass optical parametric amplification in Sec. II of the crystal, however the weak component at around 3.87 μm appears to be more easily attributed to the longer idler band linked to the 1.08- μm signal generated in Sec. I.

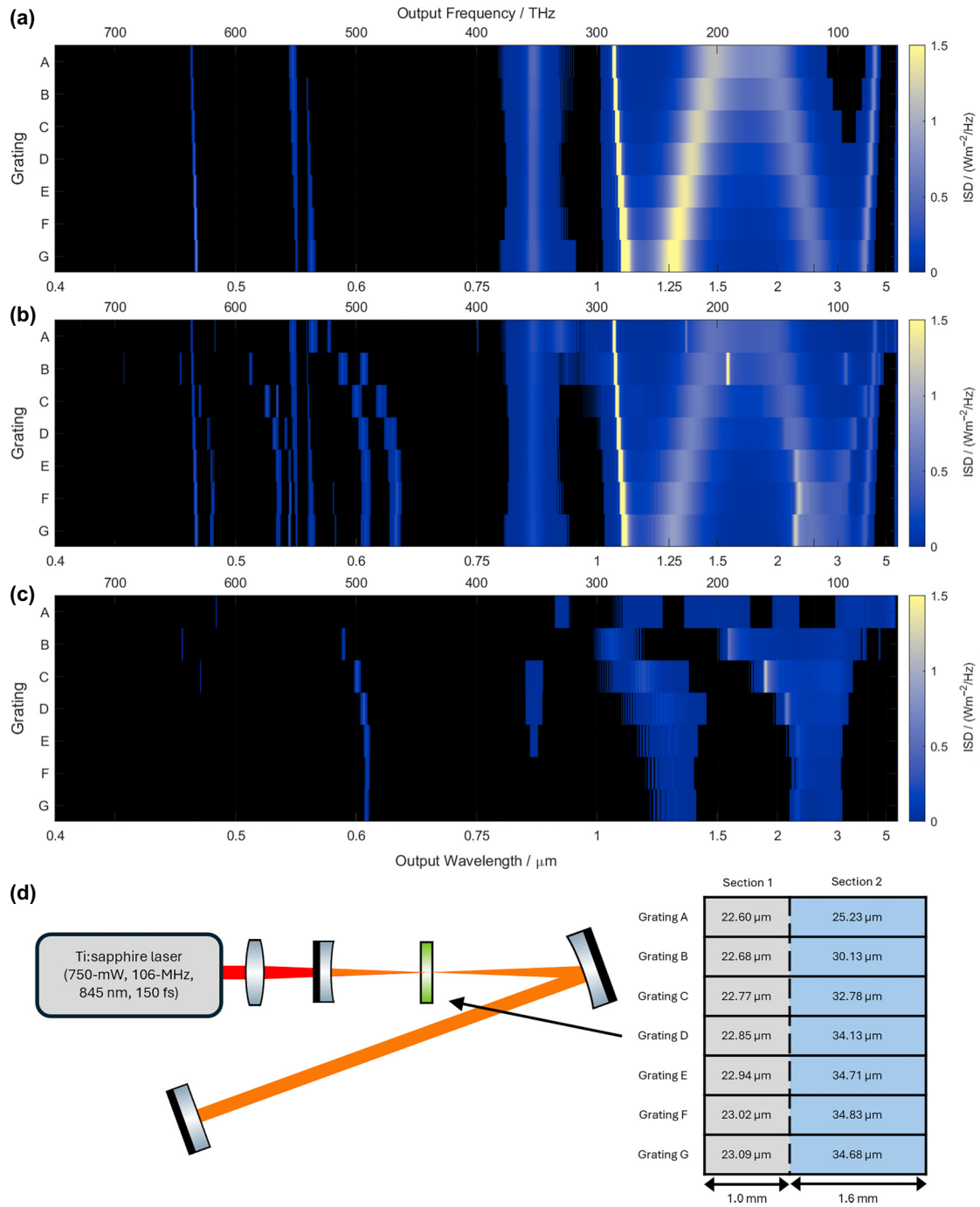


FIG. 13. (a) SCEM for crystal Sec. I pumped by the Ti:sapphire laser. (b) SCEM for crystal Sec. II, with the full SCEM from Sec. I acting as the pump source. (c) SCEM for crystal Sec. II, pumped in the reverse orientation by the Ti:sapphire laser, and the resonant idler from Sec. I. (d) Reproduction of the OPO cavity setup shown in Fig. 3 of Tillman *et al.*, [22], with laser characteristics and crystal grating periods shown for reference.

The full SCEM for the tandem OPO is shown in Fig. 13(b), where we can see enhancement at both idler and idler(2) wavelengths. A strong phase-matching region remains at around 1.2 μm , and this was observed experimentally in Ref. [22] as enhanced SHG of the primary idler. The authors also observed unexpected weak tandem

operation when the crystal orientation was reversed, which they attributed to group-velocity matching of the signal and idler in Sec. I; with small amounts of signal being converted to idler and idler(2) despite not being directly phase matched. In Fig. 13(c) we show the SCEM for the second section when placed in reverse orientation.

Here the pump is a combination of the Ti:sapphire laser and the resonant idler generated in the first section, after applying a spectral filter as defined by the cavity, reflectivity. This map shows SHG of the primary idler, generating frequency components, which are within the expected signal band of Fig. 13(a). Subsequent cascaded DFG then allows formation of a small amount of idler(2), resulting in weak tandem operation. We believe this provides a more convincing explanation for the behavior observed with the crystal in the reverse orientation, especially given the lack of relevant cascaded DFG in Fig. 13(a).

V. CONCLUSION

In summary, spectral-crystal efficiency mapping (SCEM) is introduced as a practical and powerful analytical tool for calculating potential quasi-phase-matched interactions in nonlinear media. By accounting for frequency-dependent nonlinearity, measured pump spectral profiles, and cascaded higher-order interactions, SCEM overcomes many limitations of traditional sinc-squared gain models, offering a more nuanced and accurate depiction of frequency-conversion processes.

A key feature of SCEM lies in the ability to visualize multivariate data in a single, unified representation, significantly simplifying the analysis of phase-matching potential. Previously, designing a system for QPM required simultaneous use of multiple, complex plots to understand the interactions between pump spectra and output wavelengths across a range of grating periods. SCEM consolidates this information into intuitive and comprehensive efficiency maps, providing an immediate overview of a system's spectral potential. These maps can be applied directly to traditional fan-out grating structures, but can equally be used as a starting point in the design of chirped poled waveguides [23,24]. This innovative visualization capability not only enhances clarity, but also accelerates the design and optimization of nonlinear optical systems.

The practical applications of SCEM extend across a wide range of scientific and industrial fields, including the development of broadband frequency combs, the optimization of joint spectral amplitudes [25,26] and even modulated nonlinearity for spectral engineering [27]. This last example is made possible by the ability to swap the sinc-squared function for another analytical function, corresponding to the Fourier transform of the engineered nonlinearity profile. The ability to create baseline crystal efficiency maps for a range of commonly used materials, which can be reused across diverse input spectra and system configurations, represents a significant advancement in cost-effective and time-efficient nonlinear optical modeling. It is worthwhile to emphasize that SCEM is deliberately phase agnostic: by excluding spectral phase and temporal dynamics, the method provides a global overview of the conversion landscape that complements,

rather than competes with, phase-sensitive numerical simulations. The resulting maps guide both computational and experimental efforts and should serve to simplify the early stages of experimental design, as well as the inevitable troubleshooting diagnostics of real-world optical systems.

Future work will aim to refine SCEM further by incorporating nonideal crystal structures and exploring its adaptability to different nonlinear regimes and engineered grating designs. As previously noted, the sinc-squared function can be replaced with more elaborate mathematical formulations, leaving the rest of the SCEM methodology unchanged. This leaves room to incorporate additional factors into the process, such as a variable interaction strength due to changes in spatial mode overlap. By continuing to bridge the gaps between analytical models, numerical models, and empirical data, SCEM provides a platform for collaborative development of evolving reference libraries. Such exemplar plots should allow crystal manufacturers to transparently convey the capabilities of their products, whilst enabling researchers to adopt a more modular approach to the development of alternative frequency-conversion devices.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

The data that support the findings of this article are openly available [15,16].

APPENDIX A: COUPLED-WAVE EQUATIONS AND THE SINC-SQUARED FUNCTION

We start from the coupled-wave equations derived in Sec. 2.2 of Boyd [1]. Working under the slowly varying envelope approximation, we have

$$\frac{dA_3}{dz} = \frac{2id_{\text{eff}}\omega_3}{n_3c}A_1A_2e^{i\Delta kz}, \quad (\text{A1a})$$

$$\frac{dA_1}{dz} = \frac{2id_{\text{eff}}\omega_1}{n_1c}A_3A_2^*e^{-i\Delta kz}, \quad (\text{A1b})$$

$$\frac{dA_2}{dz} = \frac{2id_{\text{eff}}\omega_2}{n_2c}A_3A_1^*e^{-i\Delta kz}, \quad (\text{A1c})$$

where the amplitudes of A_1 and A_2 are constant; A_3 is a slowly varying function of distance z ; $\omega_3 > \omega_2 \geq \omega_1$ are angular frequencies; n_j is the refractive index of the nonlinear medium at ω_j ; and d_{eff} is the effective nonlinear

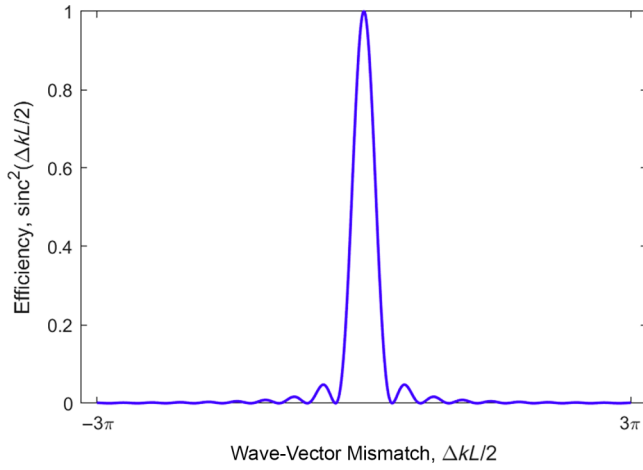


FIG. 14. Effects of wave-vector mismatch on the efficiency of SHG.

coefficient. The wave-vector mismatch between the waves is

$$\Delta k = k_1 + k_2 - k_3. \quad (\text{A2})$$

For certain conditions, $\Delta k = 0$ and the amplitude of A_3 in Eq. (A1a) increases linearly with z and so intensity I_3

increases quadratically with z . This condition is known as **perfect phase matching**. Generally $\Delta k \neq 0$ and so the amplitude of A_3 increases less than linearly with z . We can find the amplitude of A_3 by integrating Eq. (A1a) from $z = 0$ to $z = L$ to get

$$\begin{aligned} A_3(L) &= \frac{2id_{\text{eff}}\omega_3 A_1 A_2}{n_3 c} \int_0^L e^{i\Delta k z} dz \\ &= \frac{2id_{\text{eff}}\omega_3 A_1 A_2}{n_3 c} \left(\frac{e^{i\Delta k L} - 1}{i\Delta k} \right). \end{aligned} \quad (\text{A3})$$

The intensity of wave ω_3 is given by the magnitude of the time-varying Poynting vector:

$$I_j = 2n_j \epsilon_0 c |A_j|^2, \quad j = 1, 2, 3, \quad (\text{A4})$$

therefore the intensity of the generated wave is

$$I_3 = \frac{8n_3 \epsilon_0 d_{\text{eff}}^2 \omega_3^2 |A_1|^2 |A_2|^2}{n_3^2 c} \left| \frac{e^{i\Delta k L} - 1}{\Delta k} \right|^2. \quad (\text{A5})$$

The squared modulus term at the end of Eq. (A5) can be rewritten as

$$\left| \frac{e^{i\Delta k L} - 1}{\Delta k} \right|^2 = L^2 \left(\frac{e^{i\Delta k L} - 1}{\Delta k L} \right) \left(\frac{e^{-i\Delta k L} - 1}{\Delta k L} \right)$$

ALGORITHM 1. SCEM: A single-process (SHG) overview including the intensity limit.

Require: Nonlinear crystal, X , pump intensity spectral density $\tilde{I}_p$, sample frequencies ω , choice of nonlinear process

Ensure: Spectral crystal efficiency map *SCEM*

- 1: **Generate possible output frequencies:**
 - 2: $[\omega_{\text{SFG}}, \text{index}_{\text{SFG}}] \leftarrow$ sum frequency generation grid (ω, ω') ▷ Indices correspond to the position of ω_{SFG} in ω
 - 3: **Get material-dependent arrays:**
 - 4: $n_r \leftarrow X.\text{Refractive-Index}(\omega)$ ▷ From Sellmeier equation
 - 5: $k \leftarrow$ input angular wave numbers
 - 6: $k_{\text{SFG}} \leftarrow$ output angular wave numbers
 - 7: **Calculate conventional sinc² quasi-phase-matching grid:**
 - 8: $dk_{\text{SFG}} \leftarrow |k + k' - k_{\text{SFG}}|$ ▷ Absolute wave-number mismatch grid
 - 9: **for** each grating period Λ in X **do**
 - 10: $dk_{\text{QPM}}(\Lambda) \leftarrow dk_{\text{SFG}} - 2\pi/\Lambda$ ▷ Crystal adjusted, wave-number mismatch grid
 - 11: $Q(\Lambda) \leftarrow \text{sinc}^2(dk_{\text{QPM}}(\Lambda) * X.\text{Length}/2)$
 - 12: **for** relevant higher order terms m **do** ▷ For idealised $\chi^{(2)}$, $m = 3, 5, 7 \dots$
 - 13: $dk_{\text{QPM}}(\Lambda) \leftarrow dk_{\text{SFG}} - 2m\pi/\Lambda$ ▷ $[\text{m}^{-1}]$
 - 14: $Q(\Lambda) \leftarrow Q(\Lambda) + \text{sinc}^2(dk_{\text{QPM}}(\Lambda) * X.\text{Length}/2)/m^2$ ▷ Combined phase-mismatch operator
 - 15: **end for**
 - 16: **end for**
 - 17: **Calculate power-conversion efficiency grid:**
 - 18: $d_{\text{eff}} \leftarrow X.\chi^{(2)}/\pi$ ▷ $[\text{mV}^{-1}]$
 - 19: $P_\eta \leftarrow 2d_{\text{eff}}^2 \omega_{\text{SFG}}^2 / n_r[\omega] n_r[\omega'] n_r[\omega_{\text{SFG}}] \epsilon_0 c^3$ ▷ $[\text{W}^{-1}]$
 - 20: **Create process's spectral filter:** ▷ The exact form varies by process
 - 21: $S \leftarrow \tilde{I}_p \tilde{I}_p^T * X.\text{Length}^2$ ▷ $[\text{W}^2 \text{m}^{-2} \text{Hz}^{-2}]$
 - 22: **Process SCEM**
 - 23: Combine operators $\leftarrow S P_\eta Q$
 - 24: Apply intensity limit
 - 25: Transform SCEM into output space using `binNd`
 - 26: **Return** *SCEM*
-

ALGORITHM 2. BINND: Binning Multidimensional Sparse Data (Simplified for Cell Arrays).

Require: Cell array of sparse data M , array of indices ids
Ensure: Binned data structure M_{binned}

- 1: **Initialize parameters:**
- 2: $n_z \leftarrow$ number of cells in M $\triangleright$ Corresponds to N_{Λ_G}
- 3: $n_{xy} \leftarrow$ size of the 2D sparse array in each cell of M $\triangleright$ Corresponds to $N_\omega \times N_\omega$
- 4: **Create index arrays for each dimension:**
- 5: **for** each dimension d in n_{xy} **do**
- 6: $indices[d] \leftarrow 1$ to $n_{xy}[d]$
- 7: **end for**
- 8: **Generate coordinate grids using** `ndgrid`:
- 9: $[indices[1], indices[2], \dots, indices[N]] \leftarrow \text{ndgrid}(indices[1], indices[2], \dots, indices[N])$
- 10: **Assign new indices using** ids :
- 11: $indices[2] \leftarrow ids$
- 12: **Flatten and combine indices:**
- 13: **for** each dimension d **do**
- 14: Reshape $indices[d]$ into a column vector
- 15: **end for**
- 16: $indicesMatrix \leftarrow$ concatenate $indices[1], indices[2], \dots, indices[N]$
- 17: **Prepare data for GPU processing (if available):**
- 18: **if** GPU device is available **then**
- 19: **for** each element $M[z_i]$ in M **do**
- 20: Convert $M[z_i]$ to GPU array
- 21: **end for**
- 22: **end if**
- 23: **Initialize output container:**
- 24: $M_{binned} \leftarrow$ empty cell array of size n_z
- 25: **Process each data slice:**
- 26: **for** $z_i \leftarrow 1$ to n_z **do**
- 27: $M_{z_i} \leftarrow$ full array from $M[z_i]$ $\triangleright$ Convert sparse cell to full array (required for accumarray)
- 28: **Aggregate data using** `accumarray`:
- 29: $M_{binned}[z_i] \leftarrow$ sparse array created by:
- 30: – Subscripts: $indicesMatrix$
- 31: – Values: $M_{z_i}(\cdot)$
- 32: – Size: n_{xy}
- 33: – Function: `max` $\triangleright$ When multiple elements share an index, take the maximum value
- 34: **if** Data is on GPU **then**
- 35: **Retrieve data from GPU:**
- 36: Gather $M_{binned}[z_i]$ back to CPU
- 37: **end if**
- 38: **end for**
- 39: **Return** M_{binned}

$$\begin{aligned}
&= 2L^2 \frac{(1 - \cos(\Delta kL))}{(\Delta kL)^2} \\
&= L^2 \frac{\sin^2(\Delta kL/2)}{(\Delta kL/2)^2} \\
&= L^2 \text{sinc}^2(\Delta kL/2). \tag{A6}
\end{aligned}$$

Finally, an expression for I_3 can be written in terms of I_1 and I_2 using Eq. (A4) to yield

$$I_3 = \frac{2d_{\text{eff}}^2 \omega_3^2 I_1 I_2}{n_1 n_2 n_3 \epsilon c^3} L^2 \text{sinc}^2(\Delta kL/2), \tag{A7}$$

where the wave-vector mismatch Δk is contained entirely within the sinc^2 term. This mismatch factor is plotted in Fig. 14.

APPENDIX B: ALGORITHM DETAILS

A broad overview of the SCEM process is given in pseudocode in Algorithm 1. For the full SCEMs shown in Sec. III, the frequency grid was $2^{13} \times 2^{13}$ points, and the fan-out grating was sampled at 201 values of Λ_G .

1. Setting power limits for SCEM

If the intensity spectral density of one or both of the input fields is well known at the start of the crystal (as

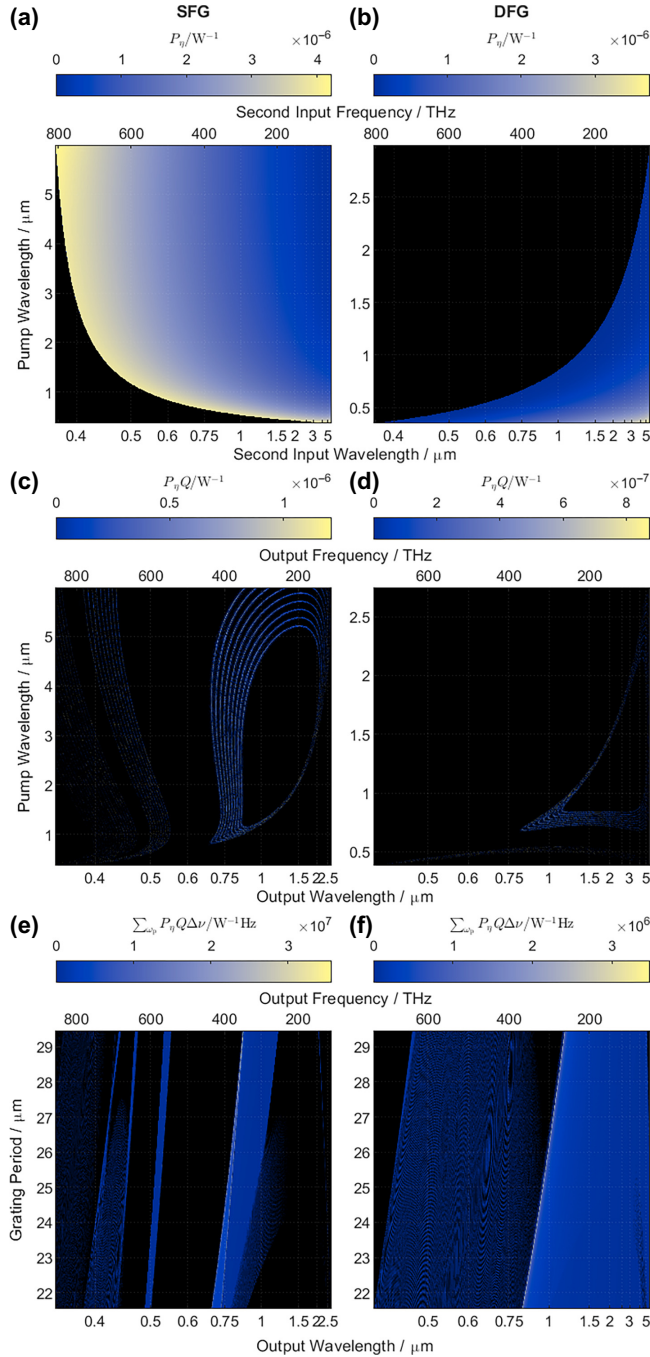


FIG. 15. PPKTP conversion efficiency for (a) SFG and (b) DFG processes. Sample grating QPM curves from $\Lambda = [27.5 - 32.5] \mu\text{m}$ for (c) SFG, (d) DFG. Crystal-only efficiency maps for (e) SFG and (f) DFG.

might be the case for a well-characterized single-pass system), the SCEM algorithm can be leveraged to find the maximum potential output intensity for each spectral component. This by no means suggests that such a result is achievable in a real system, but it does serve as a useful reality check. More pertinently, it can quickly identify parts of the spectrum, which will be inefficient to

access with a given system, regardless of how well optimized it might be (as per the original inspiration for this work). To do this, we need to apply some form of limit to $\tilde{I}_{\text{out}}(\omega_1, \omega_2, \Lambda)$, based on the magnitude of the spectral filter function, $S_{\Lambda}(\omega_1, \omega_2)$, which will mitigate some of the inconsistencies caused by the conventional undepleted pump approximation.

Setting this power limit is not a simple case of ensuring that energy is conserved; in fact, since an SCEM should represent the maximum conversion efficiency for each spectral component independently, energy should generally *not* be conserved across the whole map. This is indicative of the ability to tune experimental parameters in order to maximize gain in a chosen spectral region, such that the majority of the converted power is kept in a relatively narrow band. As such, the absolute upper limit on each SCEM element must represent the idealized case where all of the relevant input power is used to generate that single frequency (whilst remaining consistent with the process's other efficiency and phase-matching constraints).

For a single-pass system, the limit is calculated by normalizing the spectral filter, $S_{\Lambda}(\omega_1, \omega_2)$ relative to the crystal length, L , and the larger intensity of the two input fields, resulting in a map of the minimum intensity spectral density at each combination of input frequencies, which can be used to limit $SP_{\eta}Q$.

$$SP_{\eta}Q = \min \left(SP_{\eta}Q, \frac{S/L}{\max(I_1, I_2)} \right). \quad (\text{B1})$$

This should prevent individual processes (e.g., pump SHG) from scaling infinitely and make the SCEM much more useful for optimizing design parameters (e.g., matching crystal length to input power). If the system being modeled is seeded from background states (OPG, OPO), then we cap at the maximum ISD of the two fields, rather than the minimum, to allow for the fact that the background is not “depleted” in the same way as other input fields.

2. Transformation onto a common basis

In order to provide intuitive visualization of phase-matching efficiency, it is necessary to plot potential intensity as a function of resultant (as opposed to input) wavelength (frequency). This is central to producing an easily parsable image, conveying output spectral intensity, for a range of crystal gratings simultaneously. For a single nonlinear process, this is a straightforward task; conservation of energy dictates the potential photon frequencies, independent of grating period, so one simply uses the calculated phase-matched component values in place of the secondary input (x) axis. The allowed output frequencies will, however, vary by process, so adding the results of multiple processes into a single field requires manipulating the arrays so that values with the same index correspond to the same frequency. The issue is exacerbated by the fact

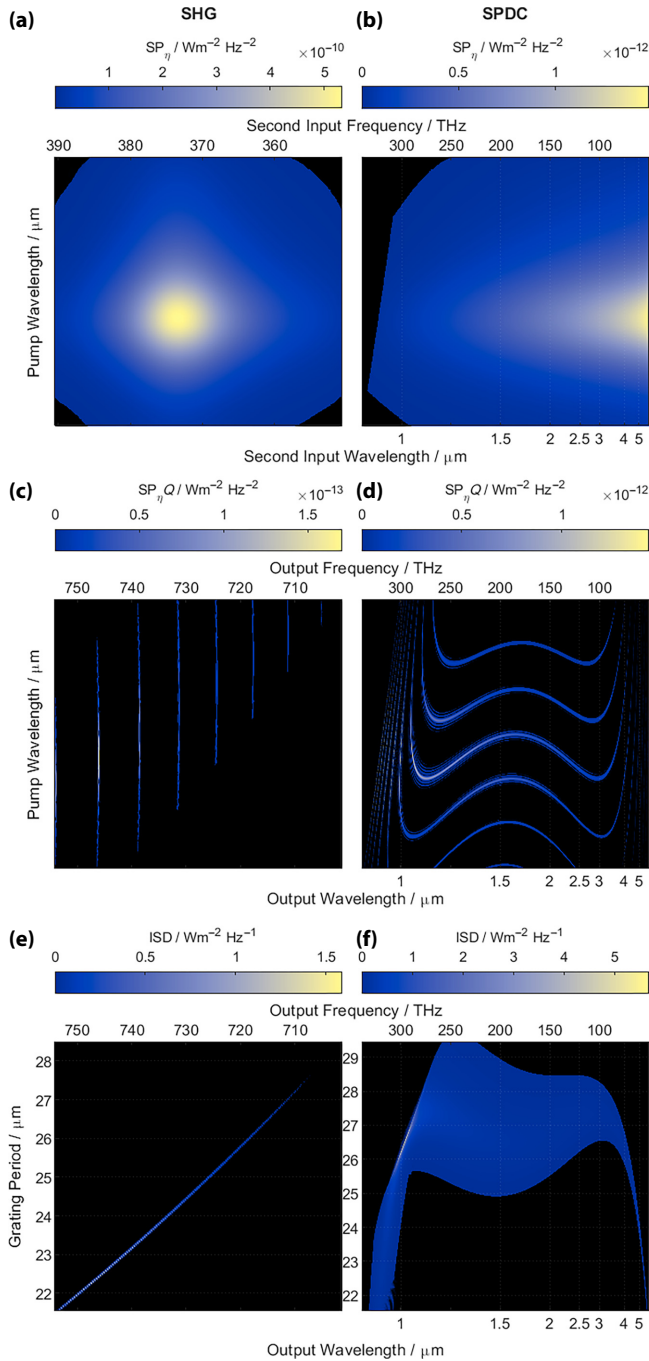


FIG. 16. Pump-weighted conversion efficiency for (a) pump SHG, (b) SPDC. Sample grating QPM curves from $\Lambda = [27.5 - 32.5] \mu\text{m}$ for (c) pump SHG, (d) SPDC. SCEM for (e) pump SHG and (f) SPDC.

that multiple components in a single output field will correspond to the same resultant frequency, and these values must be weighted individually, before being accumulated as part of the transformation.

The frequency domain must be the same for every step in the algorithm, and it must account for all potential frequency-conversion processes within the transparency

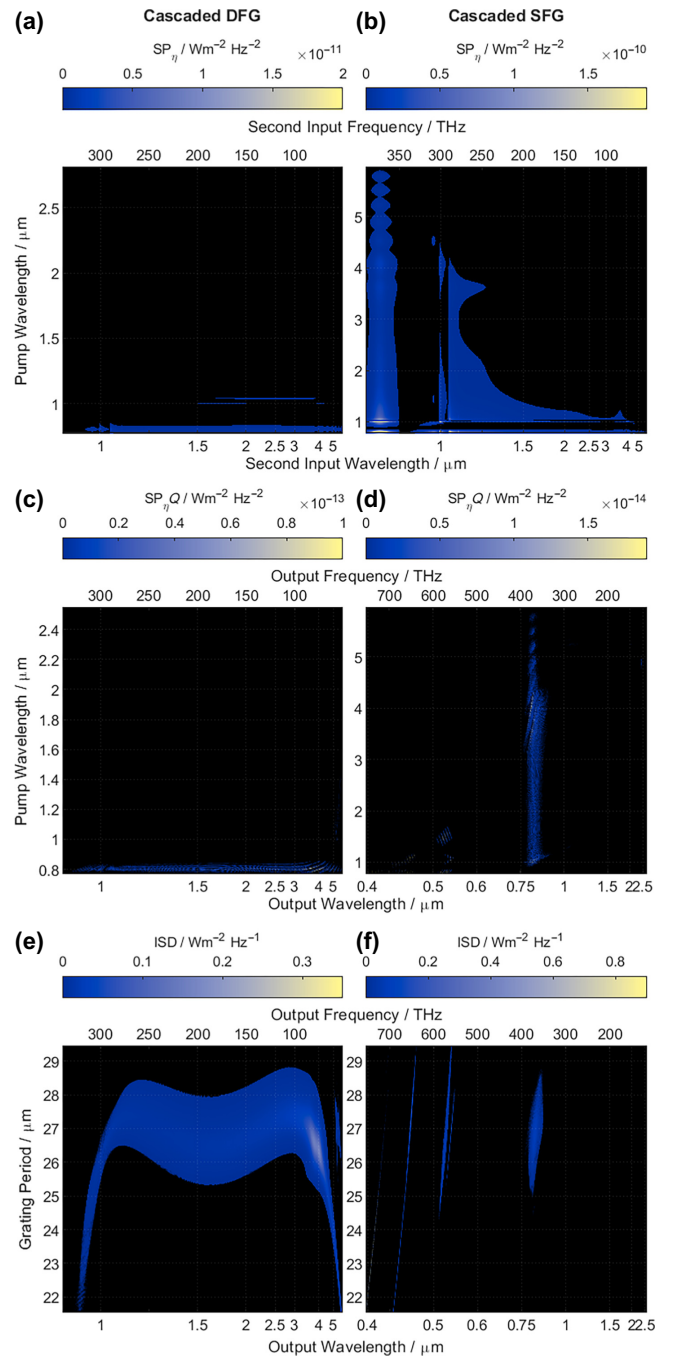


FIG. 17. Cascaded conversion efficiency weighted by initial SPDC for (a) DFG, (b) SFG. Sample grating QPM curves from $\Lambda = [27.5 - 32.5] \mu\text{m}$ for (c) DFG, (d) SFG. Additional SCEM for cascaded (e) DFG and (f) SFG.

window of the chosen crystal. As such, each individual process will result in relatively few nonzero intensities, and sparse arrays must be used if the algorithm is to feasibly be performed using local memory. Since MATLAB only supports sparse arrays in 2D, the QPM data for each sample grating is stored in a cell array, and a custom function (Algorithm 2) is required to bin these data according

to output frequency index. The crystal-only QPM array retains its original shape so that the SCEM for each process (binned according to the output frequency) can be used as an input filter, before again transforming the result into a cascaded SCEM represented on the common basis.

APPENDIX C: SCEM PLOTS FOR PPKTP

Here we provide plots of PPKTP crystal-only efficiency maps (Fig. 15), SCEMs for pump SHG and SPDC (Fig. 16), and cascaded SCEMs for DHG and SFG processes (Fig. 17).

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