Parameter Estimation of an Ion-Exchange Process Based on a Pseudo Probability Measure

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***Abstract*—For the realization of integrated optical waveguide components, needed for integrated photonic circuits, a promising approach to manufacturing is their embedding in thin glass sheets by thermal diffusion processes. Because prototyping or manufacturing small batch series is costly, appropriate numerical simulations are used in order to allow an accurate characterization. However, in practical applications it is often more interesting to estimate the parameters of the manufacturing process based on specific features of the components. In this work, an estimation approach for these parameters is proposed and evaluated.**

I. Introduction

For manufacturing integrated waveguide components by diffusion, a metallic mask is grown on the substrate material. The immersion in an ionic salt melt results in a characteristic change of silver ion concentration in the areas of the mask opening and, thus, an altered refractive index [1]. With a given set of process parameters the ion-exchange process can be accurately modeled by Fick's law. Although semi-analytic modeling approaches help with the forward simulation [2], [3], three-dimensional simulations remain both resource and time intensive. However, practical applications more often require the estimation of the parameters of the manufacturing based on specifically desired features.

The forward simulation provides a fundamental understanding of the manufacturing process and the influence of the according process parameters [3], [4]. Any specifically defined feature, e.g. geometrical or optical, can be derived from simulation results.

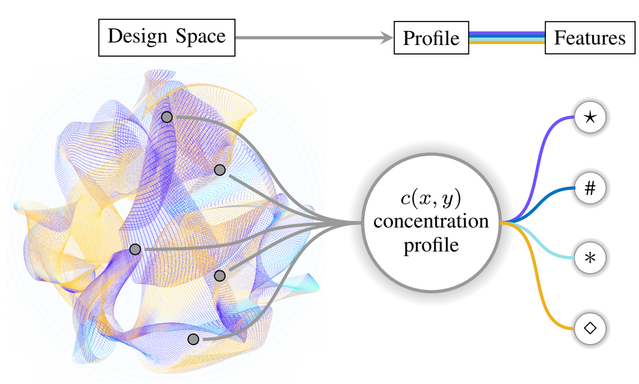

Fig. 1. With a chosen set of process parameters the multivariate design space is mapped onto the co-domain, the concentration profile. The characterization of the profile itself yields the relevant features.

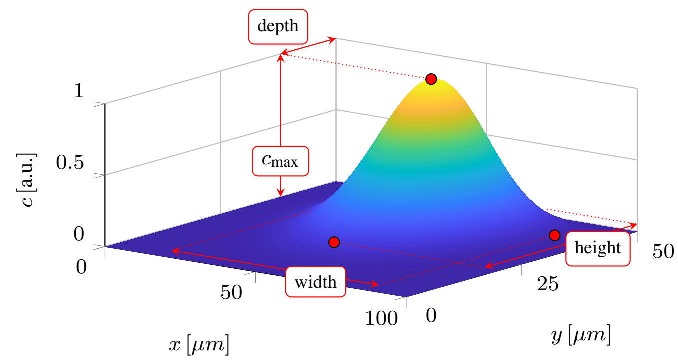

Fig. 2. Exemplary concentration profile and the defined features for the purpose of parameter estimation, which are maximum concentration $c_{\max}$, diffusion depth at $c_{\max}$ as well as height and width of the profile.

II. Feature Extraction and Parameter Compression

Specific component features result from the requirements of the application. The necessity to ensure that all requirements are met introduces difficulties because the design space of the diffusion process is too large to find the right parameter combination by sweeping through a sufficient and representative number of combinations. Therefore, an accurate estimation of the appropriate process parameters is essential. Figure 1 depicts the multivariate design space. A chosen set of process parameters yields the according concentration profile from which relevant features can be derived. This leads to a fundamental problem because the non-linear saturation effects of the diffusion process create ambiguities in feature characterization. In other words, the mapping from design space onto the co-domain is not bijective and multiple combinations of process parameters can and do result in matching features. The features used for the purpose of parameter extraction are shown in Figure 2. The profile is therefore characterized by its maximum concentration $c_{\max}$, the diffusion depth at $c_{\max}$ as well as by its height and width. Furthermore, the process parameters of the diffusion process are the initial concentration of silver ions in the salt melt c_0, diffusion times t_{in}, t_{out} and the mask width w.

The basis for the estimation is the determination of the dependencies between waveguide features and process parameters, which can be done with a small, limited number of sim-

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ulations. In general, these dependencies are ambiguous and, therefore, a single feature is not sufficient for the estimation of all parameters. The feature extraction results in a four-dimensional matrix per feature. In the first step, two process parameters are selected as primary - in this case the diffusion times t_{in} and t_{out}, which were chosen because their combination is the most ambiguous [5]. Then, the feature matrices are fit over these primary parameters, which is equivalent to an interpolation. The dependencies can be accurately represented by a polynomial fit. This simplicity is beneficial. Furthermore, the resulting coefficients of the polynomial fit can be fitted again over the remaining two secondary process parameters c_0 and w. This has one essential benefit, since the estimation model is no longer depending on the number of supporting points of the initial simulation. This double-fit approximation can be interpreted as a parameter compression. Each feature is now represented by only a small number of coefficients.

III. Parameter Estimation

The estimation of the process parameters is done by evaluating the compressed model reversely. The four-dimensional feature dependencies are generated with the function of the fits and the according coefficients of the compressed double-fit model. At this point, a testing set of known or desired feature values is provided. For each feature and all combinations of secondary process parameters a deviation σ_p is calculated as a function of the primary process parameters, which describes a difference between generated feature value and testing set. Further, this deviation is used to compute a pseudo probability measure p_p:

$$p_p(t_{\text{in}}, t_{\text{out}}) = \frac{1}{\sqrt{2\pi}\,\sigma_p(t_{\text{in}}, t_{\text{out}})} e^{-\frac{1}{2}\left(\frac{1}{\sigma_p(t_{\text{in}}, t_{\text{out}})}\right)^2} \qquad (1)$$

Hence, the more the modeled feature value and the value of the testing set diverge the higher the deviation σ_p becomes resulting in a smaller probability for this particular combination of process parameters. When the probabilities for each feature and all combinations of secondary process parameters are calculated they are normalized and superposed. By the means of this superposition of feature probabilities the most probable combination of primary process parameters is found.

Figure 3 shows the distribution of the pseudo probability measure for a testing set of feature values. As can be seen, a maximum probability of 82.68% occurs at the correct corresponding combinations of process parameters. The marked artifacts only occur in the immediate neighborhood of the maximum and are caused due to parameter compression by fitting. Benchmarks of the estimation show that the correct combinations of process parameters are identified unambiguously with a probability of over $80\,\%$ for both, the original supporting points of the forward simulation and the interpolated ones of the double-fit approximation. Interestingly, this estimation approach identifies all primary and also all secondary process parameters correctly by only evaluating a probability measure for the primary process parameters t_{in} and t_{out}, which is not self-evident. This is because of the way the features relate

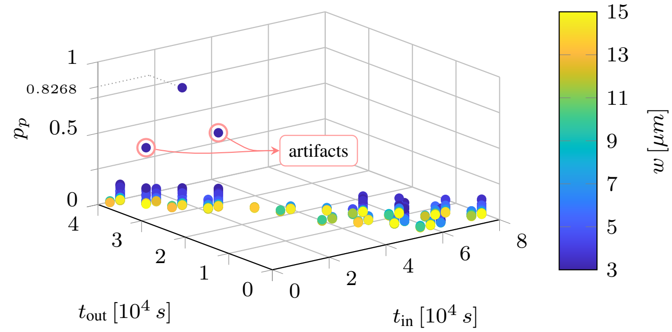

Fig. 3. Pseudo probability measure p_p depending on all primary and secondary process parameters t_{in}, t_{out}, w and c_0. Numerical compression artifacts are marked.

to the process parameters. The only nonlinearity in these relations is the saturation effect of the maximum concentration. Additionally, the type of visualization in Figure 3 also reveals different clusters of potential solutions if similarly probable. If an unambiguous identification is not possible, the combinations of primary and secondary process parameters can be permuted in order to evaluate additional, possibly different relations for a distinct identification without having to extend the scope of the forward simulation.

IV. Conclusion

The estimation of the process parameters of the thermal ion-exchange process yields excellent results with respect to the unambiguous estimation of primary and secondary process parameters. The relations between characterized features of the concentration profile and the primary process parameters greatly benefit the simplification of the estimation process. Furthermore, the implications of these results open up an additional approach. If certain process parameters are fixed due to specific hardware of other external specifications the subspace of remaining parameters can be estimated in order to find an optimal solution.

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