Inverse Modeling of Buried, Ion-exchanged Glass Waveguides using Adjoint Method

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***Abstract*—Inverse modeling of two-step ion-exchange processes for buried glass waveguides fabrication is presented. An adjoint method based approach has been used to evaluate the Jacobian matrix of the model and shown its advantages to the finite difference method.**

I. Introduction

Optical interconnects on board-level are playing an important role while the high-bandwidth and high-performance information channels are more in demand nowadays but the conventional electrical interconnects are limited by signal integrity problems. Several methods [1], [2], [3], [4] have been developed for integrating optical interconnects into electro-optical printed circuit boards (EOCB) and showed their advantages in contrast to the conventional interconnects. Because of the compatibility with single- and multimode optical fibers, more attention has been paid to glass waveguides.

The ion-exchange process is a common approach for fabricating graded-index (GI) multimode waveguides in glass. Surface waveguides can be fabricated by placing thin glass sheet in a dilute salt melt (e.g. $AgNO_3$)[5]. In some applications (e.g. optical coupler and splitter) waveguides with a buried graded-index profile are expected. These can be achieved using a two-step diffusion process [6], which forms a surface waveguide in the first step and modifies it by inverse diffusion in pure $NaNO_3$-melt in the second step.

The two-step process can be modeled using Fick's law [7] with knowing process parameters like total diffusion time, diffusion coefficient of Ag^+ in salt melt and process time for the first step. A "forward modeling" refers to the determination of the relevant waveguides characteristics such as the shape of Ag^+ profile, the maximum Ag^+ concentration and its position with given process parameters. In contrast, an "inverse modeling", which refers to estimation of process parameters in order to obtain desired Ag^+ concentration profile in glass, is of great interest to industrial application. However, this two-step diffusion process is highly non-linear. An analytic solution of the inverse problem is improbable.

In this work the problem of inverse modeling of the two-step diffusion process are solved using gradient based optimization techniques. The adjoint method, which has been successfully applied in geophysics to solve a steady-state inverse problem [8], is used to evaluate the gradients of our time-dependent inverse model.

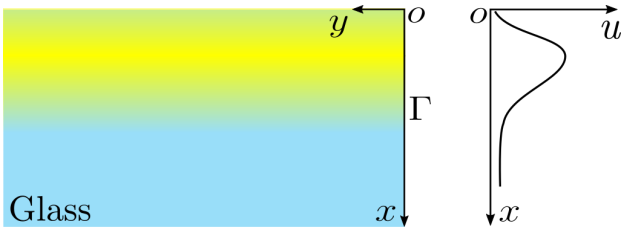

Fig. 1. Schematic representation of the process domain Γ (left) and the concentration profile u after two-step diffusion process (right).

II. Modeling

According to Fick's law the one dimensional Na^+-Ag^+ exchange process can be described with a time–dependent diffusion equation [7]. By regarding the boundary conditions (Fig. 1), the two-step diffusion process can be defined as

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}(D\frac{\partial u}{\partial x}) \tag{1a}$$

$$u_0 = 0 \qquad \text{at } t = 0, \text{ on } \Gamma \tag{1b}$$

$$u = f(t_{on}) \qquad \text{at } x = 0 \tag{1c}$$

$$\vec{n}(D\frac{\partial u}{\partial x}) = 0 \qquad \text{at } x \to \infty \tag{1d}$$

where

- State u is the normalized Ag^+ concentration in glass,
- t is the diffusing time,
- D is the self-diffusion constant of Ag^+ in glass,
- t_{on} is the diffusion time for the first step,
- $f(t_{on})$ is a modified step function:

$$f(t_{on}) = \begin{cases} 1 & t \le t_{on} \text{ (first step diffusion)} \\ 0 & t > t_{on} \text{ (second step diffusion).} \end{cases}$$

The Ag^+ concentration can be calculated by solving (1) using the Finite-Element-Method. The solution is described in more detail in [9].

Using the squared $\mathtt{L}_2$ norm, a cost function $g(t, D, t_{on})$ for solving the inverse problem of the two-step diffusion process along Γ with given target concentration profile u_{target} can be defined as

$$g(t, D, t_{on}) = \int_\Gamma (u(t) - u_{target})^2 \, \mathrm{d}x. \tag{2}$$

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An optimization procedure – Gradient descent – is used to minimize the cost function. Normally, the Jacobian matrix can be evaluated using finite difference method. However, with this method equation (1) needs to be solved twice for each model parameter. Thus calculating Jacobian matrix **J** can be very time-consuming, especially when the number of model parameter is large. Using the adjoint method after solving the adjoint partial differential equation

$$\frac{\partial \mu}{\partial t} = \frac{\partial}{\partial x}(D\frac{\partial \mu}{\partial x}) \tag{3a}$$

$$\mu_0 = 2(u(T) - u_{target}) \tag{3b}$$

$$\mu = 0 \qquad \text{at } x = 0 \tag{3c}$$

$$\vec{n}(D\frac{\partial \mu}{\partial x}) = 0 \qquad \text{at } x \to \infty\ , \tag{3d}$$

the Jacobian matrix at the final processing time T can be obtained as

$$\mathbf{J} = \begin{pmatrix} \frac{\partial g}{\partial t}\big|_T \\ \frac{\partial g}{\partial D}\big|_T \\ \frac{\partial g}{\partial t_{on}}\big|_T \end{pmatrix} = \begin{pmatrix} \int_\Gamma 2(u - u_{target})\,\frac{\partial u}{\partial t}\big|_T \,\mathrm{d}a \\ -\int_T \int_\Gamma \frac{\partial u}{\partial x}\big|_{T-t} \cdot \frac{\partial \mu}{\partial x}\big|_t \,\mathrm{d}x\mathrm{d}t \\ \int_T \frac{\partial f}{\partial t_{on}} D \frac{\partial \mu}{\partial x}\big|_{x=0} \,\mathrm{d}t \end{pmatrix}.$$

This approach is independent of the number of model parameter and needs only to run once for the forward model and once for the adjoint model.

III. Results and Discussion

An optimization routine using the Jacobian matrix has been developed to solve the inverse problem of the two-step diffusion process. The aim is to find the proper values of t, D, t_{on}, which minimize $g(t, D, t_{on})$. Fig. 2 depicts the convergence curves of $g(t, D, t_{on})$ with the model parameters during the optimization procedure. The procedure started with randomly chosen parameters. The appropriate profile is depicted in Fig. 3a with dash line. The target profile and the optimized profile, which is calculated with the converged parameters, are depicted respectively in Fig. 3a with solid line and red stars. The absolute difference between them is showed in Fig. 3b. A very good agreement between the target and optimized profile is obtained.

The one-dimensional inverse problem of the two-step diffusion process was solved using optimization technique. The Jacobian matrix for optimization was evaluated using an adjoint method based approach. With this method, the Jacobian matrix was evaluated more efficiently than with the finite difference method. The application of the adjoint method can be easily extended to solve a two-dimensional inverse problem of the ion-exchange process and it will be discussed in the following work.

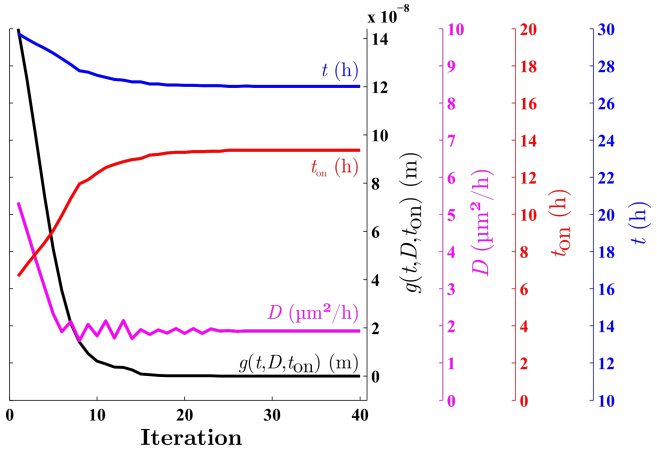

Fig. 2. Convergence curve of the cost function and model parameters during the optimization routine

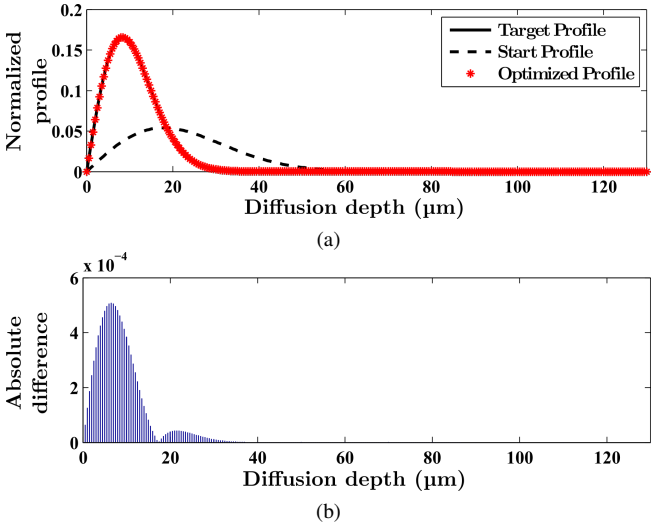

Fig. 3. Results of optimization by using Jacobian matrix **J** for the inverse design of the two-step diffusion process. The concentration profiles in (a) are normalized.

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