Neuro-Informatic Determination of Thin Film Optical Constants based on Reflection Data

Udo Trutschel[1], U. Langbein[2], M. Markert[3], M. Golz[4]
[1]DOOS Tabarz, [2]FB Physikalische Technik der FH-Wiesbaden,
[3] Institut für Physik der TU-Ilmenau, [4]FB Informatik der FH-Schmalkalden
mailto:utrutschel@doos.de

In a preliminary study an Error Back Propagation Network (EBPN) has been applied for the determination of optical constants of thin Palladium films using reflectometric and ellipsometric data sets as network inputs. First results based on angle scan data sets confirm that EBPN is a viable tool for solving the inverse problem of determining thin film optical parameters.

1 Introduction

The determination of optical thin film parameters from reflectometric and ellipsometric data sets is a basic task in material characterization. Typically, a shooting and matching technique with the optical thin film parameters as fit parameters is used to minimize the difference between simulated and measured reflectometric and ellipsometric signals.

In this paper a different method involving neural networks is presented to solve the problem of thin film parameter determination.

2 Method

Error Back Propagation Networks (EBPN's) are known for their ability of model free nonlinear function approximation [1]. This ability is based on the information processing activity in each single unit (neuron) forming a network of different unit layers as shown in **Figure 1**. The signals are transferred through the network from the input to the output layer along connection links between the units. Each connection link has a specific weight, which modifies the transmitted signal. Each neuron responds to its net input (sum of all its weighted input signals) by applying an activation function (usually nonlinear) to determine its output signal. These simple rules allow EBPN's to learn highly complex, nonlinear functional relationships between different data sets.

In our specific application, an EBPN will be trained to learn the functional relationship between a **'40'** dimensional reflectometric or ellipsometric data set and a **'3'** dimensional thin film parameter data set. The performance of the final prediction ability of the EBPN will depend on the availability of sufficient training data sets associated with the thin film configuration to be determined. Our example in mind consists of a thin Palladium (Pd) film deposited on a glass substrate and characterized by a data triplet, i.e. the real and imaginary part of the dielectric constant 'Real $\{\varepsilon\}$', 'Imag $\{\varepsilon\}$' and thickness 'D' of the Pd-film. In order to generate the necessary training and test data set at **'40'** discrete incidence angle grid points ϕ_I for a fixed wavelength (λ=633 nm) the well-known matrix method [2] has been used. Each training and test data set consists of reflectometric data 'R^{TE}', 'R^{TM}' or ellipsometric data 'tan(ψ)', 'cos(Δ)' [3], abbreviated by f(ϕ_I). Each data set is associated with a concrete choice of the Pd-film parameters which have been scanned over a specific range to cover the expected experimental variations taking into account exposure to hydrogen and different deposition methods for the Pd film, see **Figure 3.**

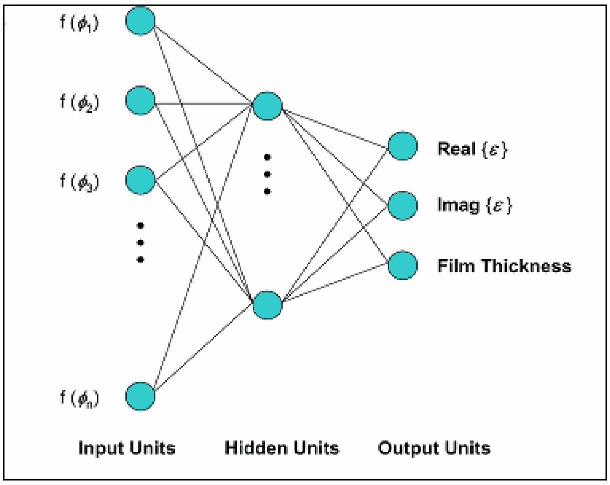

Fig. 1 *EBPN structure with '40' input units and '3' output units, f(ϕ_I) is the value the reflection data for the incidence angle ϕ_I at a fixed wavelength.*

The simulated results for '$R^{TM}(\phi_t)$ are depicted in **Figure 2**. Each triplet of real part, imaginary part and film thickness of Pd (['Real $\{\varepsilon\}$', 'Imag $\{\varepsilon\}$' and 'D']) corresponds to a star in **Figure 3** and results in **'40'** dimensional data set 'f(ϕ_i)' (i=1..40) in **Figure 2**.

Having calculated sufficient training data (blue stars in **Figure 3**) and realistic test data (green stars in **Figure 3**) the EBPN learns the correlation between the **'40'** dimensional input data set 'f(ϕ_i)' and the '**3**' dimensional target data set 't(x_j)' representing the thin film parameters triplet without further reference to a physical model. The protocol of a typical training session is shown in **Figure 4**.

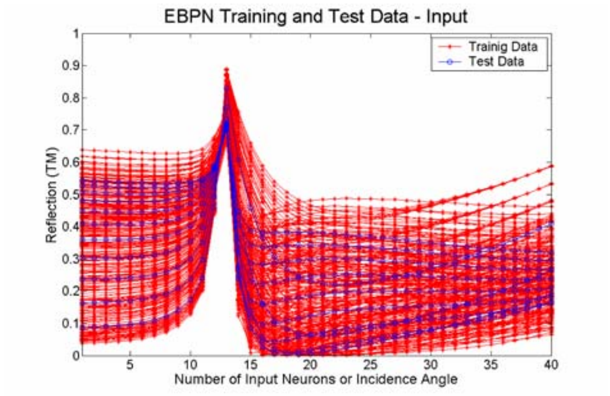

Fig. 2 Training and test data sets calculated from given triples of thin Pd film parameters

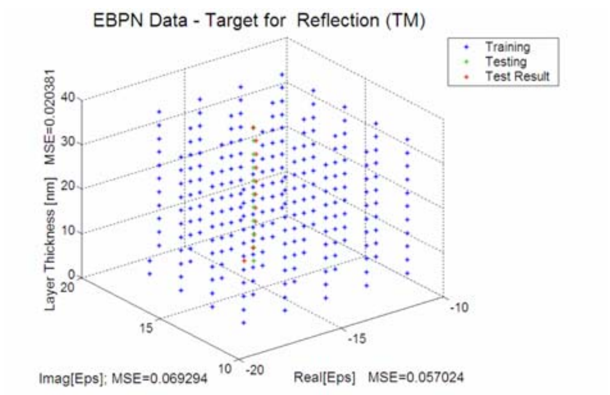

Fig. 3 The parameter cube of the optical thin Pd film parameters used to simulate training and test data sets. The axis labels show the parameter ranges chosen.

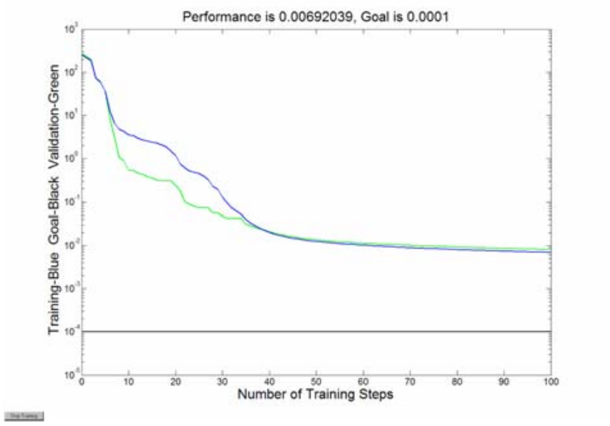

Fig. 4 Mean Square Error (MSE) versus number of training steps, the validation set has not been used for training.

After each training step the network weights are changed to reduce the difference between the EBPN response and the target function using the Mean Square Error (MSE) as error criterion. To avoid the typical overtraining of EBPN's a validation data set has been split from the training data set. This validation set has been constantly evaluated during the training process, but never used for training itself. The training should reduce the MSE between the training data (blue line in Figure 4) and the validation data (green line in Figure 4) simultaneously. If there is a succession of training steps where the MSE is reduced for the training data only and not for the validation data, a not acceptable specialization (overtraining) of the EBPN has occurred and the corresponding ill-trained network has been discarded. A properly trained network is shown in **Figure 4**.

3 Results

A test data set (blue lines, Figure 2) completely "unknown" to the EBPN with realistic optical Pd constants [4] and realistic film thicknesses has been used to test the trained network. The EBPN response is shown in **Table 1**.

	Real {ε}	Imag {ε}	D1 [nm]	D2 [nm]	D3 [nm]	D4 [nm]	D5 [nm]
Target	**-15.27**	**15.22**	**9**	**15**	**21**	**27**	**33**
Result	**-15.28**	**15.193**	**8.99**	**15.01**	**21.01**	**26.98**	**33.06**

***Tab. 1** Results from test data set, **Target** shows the thin film Pd parameter data used for calculating the input test data, **Result** gives the response of the trained EBPN.*

In **Figure 2** the Pd thin film parameters used to calculate the input test data set are denoted by target (green) and the EBPN response by result (red), respectively. **Figure 3** shows the MSE for each of the thin film parameters summarized over all test data.

The results of the angle scan confirm that EBPN are viable tools for solving the inverse problems of determining optical constants. Further research is needed to apply the proposed method to wavelength scan data sets which was described in [5]. Any simple model assumption used to approximate the dielectric function was not sufficient in the case of Palladium and led to a compromised performance of the EBPN for the wavelength scan.

Literatur

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