Characterization of nanofilm parameters based on hybrid optimization algorithm

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Abstract: In order to obtain accurate nano-film parameters in the ellipsometry measurement process, a hybrid optimization algorithm for nano-film parameter data processing was proposed. An Improved Particle Swarm Optimization-Neural Network (IPSO-NN) hybrid optimization algorithm has been proposed, based on the features of artificial neural network algorithm back propagation and particle swarm algorithm for fast optimization. This algorithm has the ability to jump out of the local optimal solution quickly with fewer iterations, so as to quickly find the optimal solution of ellipsometric equation. The algorithm was used to calculate the film parameters of silicon dioxide nano-film thickness standard template with a standard value of 26.7±0.4 nm in this paper. The results show that the relative error of the film thickness calculation by IPSO-NN hybrid optimization algorithm is less than 2%, and the refractive index error is less than 0.1. At the same time, this paper compares the traditional particle swarm algorithm with the IPSO-NN algorithm through experiments, and verifies that the IPSO-NN algorithm can optimize the number of iterations effectively and the process of finding the optimal solution. This algorithm can achieve rapid convergence and improve the calculation efficiency when calculating the thin film parameters.

Key words: ellipsometry measurement; nano-film parameters; data processing; hybrid optimization algorithm

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基于混合优化算法的纳米薄膜参数表征

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摘 要: 为了在椭圆偏振测量过程中得到精确的纳米薄膜参数,提出了一种求解纳米薄膜参数的混

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合优化算法。结合人工神经网络算法反向传播和粒子群算法快速寻优的特点,建立了改进粒子群-神经网络(Improved Particle Swarm Optimization-Neural Network,IPSO-NN)混合优化算法。该算法在较少的迭代次数下具有快速跳出局部最优解的能力,从而快速寻找椭偏方程最优解。文中使用该算法对标称值为(26.7±0.4)nm 的硅上二氧化硅纳米薄膜厚度标准样片进行薄膜参数计算。结果表明:采用 IPSO-NN 混合优化算法计算薄膜厚度时相对误差小于 2%,折射率误差小于 0.1。同时,文中通过实验对比了传统粒子群算法与 IPSO-NN 算法, 验证了 IPSO-NN 算法计算薄膜参数时能有效优化迭代次数和寻找最优解的过程,实现快速收敛,提高计算效率。

关键词: 椭圆偏振测量; 纳米薄膜参数; 数据处理; 混合优化算法

0 Introduction

With the wide application of nano-film technology in the semiconductor industry, the accurate measurement and characterization of the optical constant and thickness of the film surface has become the key technology for thin films [1-3]. Ellipsometry is one of the most sensitive methods for optical parameter characterization of thin film materials. It is widely used in many industries for its high precision, non-destructive, and measurement environment independent of vacuum. Since the ellipsometric angle measured by the ellipsometer is related to the thickness and optical constant of the film, the ellipsometric equation is a nonlinear transcendental equation, and the analytical solution cannot be directly obtained [4]. Therefore, in order to obtain high-precision film complex refractive index and thickness parameters, a special algorithm is needed to perform data processing on the ellipsometry. At present, good results have be achieved by simulated annealing algorithm, genetic algorithm, particle swarm algorithm and ant colony algorithm. Among them, particle swarm optimization algorithm is widely used in film parameter inversion calculation because of its adaptability and high precision[5-7]. However, the particle swarm optimization algorithm is prone to premature convergence, especially when dealing with more complex problems, and it is easy to fall into the local optimal solution, which leads to the deterioration of the optimization ability, and affecting the calculation accuracy of the film parameters.

An Improved Particle Swarm Optimization-Neural Network(IPSO-NN) hybrid optimization algorithm has been proposed in this paper. This algorithm solved the optimal solution of ellipsometric equation by predicting the film parameters of neural network model, which combined the BP neural network´s ability to predict nonlinear equations with the particle swarm algorithm′s ability to optimize weights and thresholds. This algorithm makes up for the defect of the traditional particle swarm optimization algorithm which is easy to fall into local optimum when seeking the optimal solution. This algorithm can improved the accuracy of nano film thickness and optical constant in ellipsometry, it was applied to a variety of nano-transparent monolayer films to verify their effectiveness. Experiments show that the IPSO-NN model is used to solve the thickness of the film with a relative error less than 2%.

1 Theory summary

1.1 IPSO-NN hybrid algorithm

The particle swarm optimization (PSO) algorithm was proposed by Kennedy and Eberhar. It can be used to solve optimization problems by stimulating the food-seeking behaviors by birds[8]. This algorithm has great advantages, such as positive feedback, global optimum capacity and easily integrated with other algorithms. The principle of the algorithm is to simulate each potential optimal solution into a bird as a "particle". The particles fly at a certain speed in the search space, and their flight speed is adjusted by the group dynamically. After several iterations, an eligible food source will be found. So the particle parameters corresponding to the best position that can be preyed are searched.

This paper increases the dynamic inertia weight of particles to select the weights and thresholds in artificial neural networks accurately, based on the iterative optimization of traditional PSO algorithm, then establish an IPSO-NN model. The film parameters were modeled and calculated. The least squares principle is used to fit the calculated and experimental values of the model. Finally, the root mean square function is used to evaluate the optimal value, and the optimal value of the film parameters is output. The IPSO-NN hybrid optimization algorithm not only makes full use of the global search ability of the PSO algorithm, but also maintains the characteristics of error back propagation in the artificial neural network algorithm, and can obtain the film parameters with higher calculation accuracy. The algorithm flow chart is shown in Fig.1.

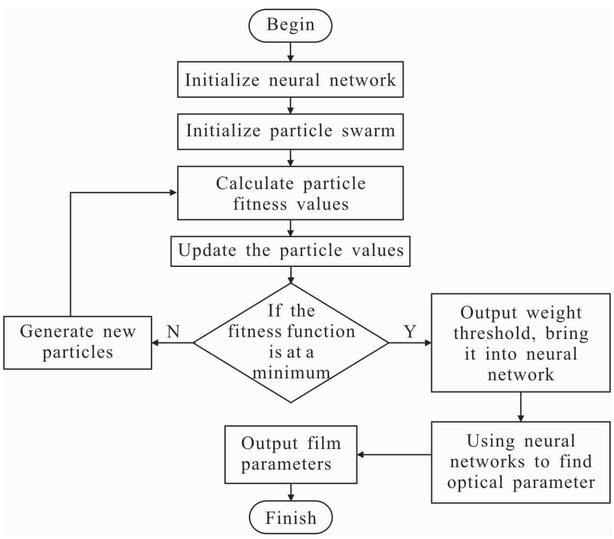


Fig.1 IPSO-NN algorithm flow chart

When the IPSO-NN algorithm is applied to ellipsometric data processing, it is first necessary to determine the input and output of the neural network algorithm, and select the training data and test data to predict and test the output. The schematic diagram of the artificial neural network structure is shown in Fig.2.

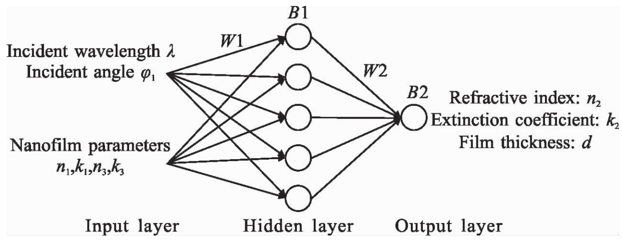


Fig.2 BP neural network structure

Where $W1$ is the weight matrix of the input layer and the hidden layer node, $W2$ is the weight matrix of the hidden layer to the output layer, $B1$ and $B2$ represent the hidden layer and the output layer respectively. Due to the different dimensions of the input and output, the data needs to be normalized so that the data is between [-1,1], which is more suitable for calculation. The normalization of the data uses the following formula:

$$x^{*}=\frac{(y_{\max}-y_{\min})\times(x-x_{\min})}{x_{\max}-x_{\min}}+y_{\min} \tag{1}$$

Where $x_{\max}$ is the maximum value in the data; $x_{\min}$ is the minimum value of the data; $y_{\max}$ is the maximum value after normalization, which is taken as 1 in this paper; $y_{\min}$ is the minimum value of the normalized data, which is taken as -1 in this paper.

Secondly, the inertia weight w of the traditional particle swarm optimization algorithm is improved to select the optimal threshold and weight for the neural network algorithm. This paper mainly changes the fixed inertia weight in the traditional PSO algorithm to the linearly decreasing inertia weight. The method of linearly reducing the inertia weight can make the PSO algorithm explore a large area in the initial stage of iteration, then reduce the iterative range and reduce the iterative speed slowly, which is convenient for the algorithm to search for the optimal solution of weights and thresholds. The improved PSO model formula is shown as below.

$$\begin{cases} v_{id}=w\cdot v_{id}+c_1r_1(p_{id}-x_{id})+c_2r_2(p_{gd}-x_{id}) \\ w=c-\lambda\cdot k \\ x=x_{id}+v_{id} \\ p_{gd}=p_{id}+v_{id}+f\cdot r_3 \end{cases} \tag{2}$$

Where v_{id} and x_{id} represent the velocity and position vector of the d dimension of the i particle, r_1 and r_2 are two independent random numbers in [0,1], c_1 and c_2 are learning factors, p_{id} is the best position of i particles which is searched in the d-dimensional search space, p_{gd} represents the global optimal position.

Finally, the weights and thresholds calculated by the PSO algorithm are brought into the artificial neural network algorithm to solve unknown film parameters. The artificial neural network algorithm model structure diagram is shown in Fig.2.

1.2 Comprehensive evaluation function

When the IPSO-NN algorithm model is used for iterative optimization, the optimal solution calculated by the model needs to be brought into the ellipsometric equation to solve the ellipsometry inversely, and the network model prediction value and experiment are solved by the least squares principle. The data values were fitted and the appropriate evaluation function was selected to evaluate the fitting results. In this paper, a function that can reflect the root mean square error gradient is selected as the evaluation function:

$$\mathrm{MSE}=\frac{1}{2K-N-1}\sum_{i=1}^{K}\left[\left(\frac{\psi_i^{\exp}-\psi_i^{\mathrm{mod}}}{\sigma_\psi^{\exp}}\right)^2+\left(\frac{\Delta_i^{\exp}-\Delta_i^{\mathrm{mod}}}{\sigma_\Delta^{\exp}}\right)^2\right] \tag{3}$$

Where $\sigma_\psi^{\exp}$ and $\sigma_\Delta^{\exp}$ are uncertainty of $\psi_i^{\exp}$ and $\Delta_i^{\exp}$, which is ellipsometric angles measured by ellipsometry, K is the number of sampling points, and N is the number of parameters that needed to be solved, ψ_i^{mod} and Δ_i^{mod} are the calculated values from ellipsometry basic Eq.(4):

$$\tan\psi\cdot \mathrm{e}^{i\Delta}=\frac{r_{1p}+r_{2p}\mathrm{e}^{-i2\delta}}{1+r_{1p}r_{2p}\mathrm{e}^{-i2\delta}}\cdot\frac{1+r_{1s}r_{2s}\mathrm{e}^{-2i\delta}}{r_{1s}+r_{2p}\mathrm{e}^{-2i\delta}} \tag{4}$$

In which, r_{1p}, r_{1s}, and r_{2p}, r_{2s} are reflectances of P and S at upper and lower interface, respectively. They can be calculated from Eq.(5).

$$r_{01p}=(N_1\cos\phi_0-N_0\cos\phi_1)/(N_1\cos\phi_0+N_0\cos\phi_1)$$
$$r_{12p}=(N_2\cos\phi_1-N_1\cos\phi_2)/(N_2\cos\phi_1+N_1\cos\phi_2)$$
$$r_{01s}=(N_0\cos\phi_0-N_1\cos\phi_1)/(N_0\cos\phi_0+N_1\cos\phi_1)$$
$$r_{12s}=(N_1\cos\phi_1-N_2\cos\phi_2)/(N_1\cos\phi_1+N_2\cos\phi_2)$$
$$2\delta=\frac{4\pi}{\lambda}\mathrm{d}n_2\cos\phi_2 \tag{5}$$

In which, N_0, N_1, N_2 are the complex refractive of air、film and substrate, respectively,ϕ_0, ϕ_1, ϕ_2 corresponding to the angle of light at the inerface, ϕ_0, ϕ_1 and ϕ_2 meet fresnel′s formula. Relationship among ϕ_0, ϕ_1 and ϕ_2 can be seen from Figure 3. N_2 and d is the complex refractive index and extinction coefficient of unknown film. For different unknown plugged N_2 and d, each value of MSE is calculated, and when MSE is zero or very hours, this pair of given N_2 and d is the parameters of the unknown thin film.

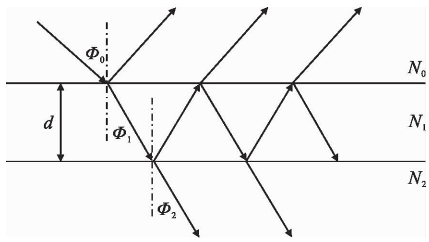


Fig.3 Reflection and refraction in the model of single-layer film

2 Simulation results and data analysis

In this paper, the model of M-2000XF spectroscopic ellipsometer manufactured by J. A. Woollam Co. was used to measure 30 nm (standard thickness is 26.7±0.4 nm, NIST) thin film thickness strandard template of silicon dioxide film thickness on silicon which were at the incident wavelength of 300-800 nm and the incident angle of 65°. The IPSO-NN hybrid optimization algorithm model is used to calculate the ellipsometric parameter. By comparing the difference between the calculated value of the model and the experimental measurement value, the optimal solution parameters of the thin film are obtained.

In reality, the surface of the top layer film and the interfaces between films usually have different n and k, and the film always are non-uniform and non-dense. Therefore, before the simulation calculation for the film parameters, the film structure should be idealized and equivalent. The equivalent structure model for SiO_2 film on Si substrate is shown in Fig.4.

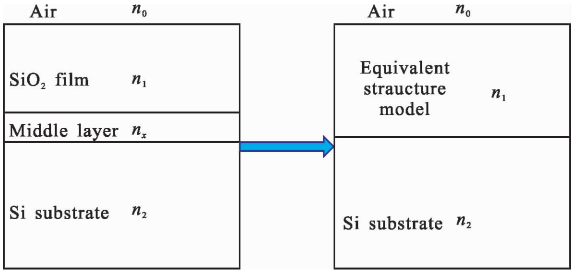


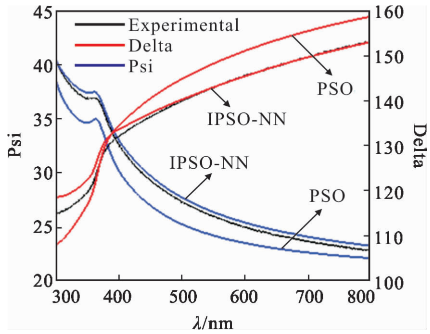
Fig.4 Model of standard samples

Secondly, the relationship between the optical constant of the film and the wavelength is established according to the difference and properties of each layer for film material. In this paper, the Cauchy's dispersion formula is used to fit the SiO_2 film, which is given in Eq.(6)[9]. In which A, B, and C are the fitting parameters, and n is the refractive index when the film at the wavelength of λ.

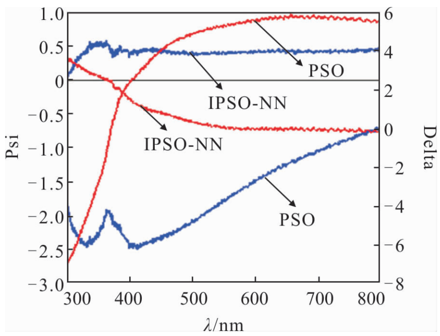
$$n(\lambda)=A+\frac{B}{\lambda^2}+\frac{C}{\lambda^4} \tag{6}$$

Although a few parameters needed to adjust in the IPSO-NN hybrid algorithm, the parameters affect the accuracy and convergence of the algorithm directly. When calculating the parameters of SiO_2 film on Si substrate, the number of particles is 20, and each particle contains three features (corresponding to refractive index n, extinction coefficient k, and film thickness d). The inertia weight has within the range of [0.4,0.9], and the learning factors are $c_1=c_2=2$.

The IPSO-NN algorithm model is used to calculate the ellipsometric parameters and thin film parameters of silicon dioxide film thickness standard samples on silicon with a nominal value of 30 nm. Through the algorithm model, the model value in the certain wavelength range has been calculated and compared with the experimental value and the calculated value of the traditional PSO algorithm. The ellipsometric parameter comparison chart is shown in Fig.5(a). The difference between the calculated results of the two algorithms and the experimental value is plotted as the error graph are shown in Fig.5(b).



(a) Ellipsometric parameters



(b) Calculation error

Fig.5 Comparison of ellipsometric parameters

From the comparison chart of ellipsometric parameters, it can be known that compared with the traditional PSO algorithm, the ellipsometric parameters of the thin film predicted by the IPSO-NN model are closest to the experimental true value in a certain wavelength range. It can be seen from the error comparison chart that the ellipsometric parameter error calculated by using the IPSO-NN algorithm in a certain wavelength range is closer to zero. When calculating the optical constants of the film, since silicon dioxide on silicon is a transparent film, the theoretical value of its extinction coefficient k is 0, and during the calculation process, it was found that as the number of iterations increases, the extinction coefficient k does not change significantly, so when solving the optical constants of the thin film, this paper mainly uses the IPSO-NN model to calculate and analyze the refractive index n of the thin film in a certain wavelength range. The relationship between the number of algorithm iterations and the thin film optical constant is shown in Fig.6.

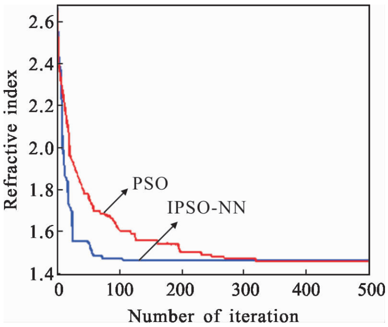


Fig.6 Comparison of algorithm convergence performance

The comparison shows that using the IPSO-NN algorithm requires fewer iterations, faster calculation speed, and easier convergence, the calculated value of the IPSO-NN algorithm is closer to the true value when calculating thin-film parameters. The optimal solution comparison data calculated using the traditional PSO algorithm and the IPSO-NN hybrid optimization algorithm are shown in Tab.1.

Tab.1 Comparison of calculation results of thickness strandard template

Film parameters	PSO algorithm	IPSO-NN hybrid algorithm
Film thickness/nm	33.40	27.10
Relative error of thickness	25.09%	1.49%
Refractive index	1.463	1.460
Extinction coefficient	0.01	0
Minimum of iterations	330	110
Minimum of MSE	4.32	3.20

The simulation results show that the IPSO-NN hybrid algorithm is more accurate than the traditional PSO algorithm, and the relative error is only 1.49%. Moreover, the IPSO-NN hybrid algorithm requires fewer iterations, and it is easier to reach a stable state when calculating the optical constant of the thin film. The IPSO-NN hybrid algorithm developed in this paper can calculate the parameters of nano films accurately and effiectively.

3 Conclusion

In this paper, an IPSO-NN algorithm model for calculating the thickness and optical constant of nano film is proposed. The algorithm can combine the advantages of PSO algorithm and artificial neural network algorithm to solve the nonlinear transcendental ellipsometric equation. In this paper, a typical nanofilm standard sample is used to calculate and analyze, which shows that the IPSO-NN algorithm can break through the traditional PSO algorithm to find the optimal solution in the calculation of film thickness inversion effectively. By comparing with the nominal values of the nanofilm standard samples, it is verified that the IPSO-NN hybrid optimization algorithm is an accurate and fast calculation method for the transparent film parameter inversion calculation process.

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