

## Quantitation of Phosphorus in a Silicon Wafer Using

As typical methods of multivariate calibration analysis, multiple-linear regression and the PLS (partial least-squares) are often applied. The multiple-linear regression can be classified into CLS (Classical Least-Squares) method and ILS (Inverse Least-Squares) method, which are applied for simultaneous determination of multiple components and for the determination of specific components among multiple

components respectively. The PLS method is notable for the solution of some problems peculiar to multiple-linear regression and for the excellent determination accuracy. In this article, examples of applying the PLS method for the determination of phosphorus and boron in silicon wafer are introduced.

### About the PLS Method

The PLS, which is an expansion of the PCA (Principal Component Analysis) method, has both the advantage of the CLS method to be able to use data of the entire wavelength range as a result of solving the problem in attaining collinearity and the advantage of the ILS that although information on concentration of all the components is not available, quantitation of a specific component is possible. Furthermore, it is known that in comparison with multiple-linear regression, it is less affected by the baseline drift or noise. In the PLS method, the following model expression is used.

$$A = TB + E \quad (1)$$

This formula, in which matrix A indicates the spectrum of the sample, is expressed by the product of a loading matrix B indicating the obtained spectrum of the components (which are not necessarily consistent with the actual components) and a score matrix T corresponding to the concentration of the components. E is a matrix showing a residual. Row vector c which shows concentration of an actual component can be expressed as follows by using the score matrix T.

$$c = T v + e \quad (2)$$

v is a row vector correlating c with T. e is a row vector representing residual.

Further, the score vector T can be expressed as follows to reflect information on the spectrum using a weight vector W.

$$T = AW \quad (3)$$

The concepts of the CLS method and ILS method are integrated in equations (1) and (2). For that reason, the PLS method has the features of both methods. In actual calculation, T, B, and v are obtained in such a way that the norm of each of E and e becomes minimal from the spectrum A of the standard sample and concentration c. NIPALS (Nonlinear Interactive Partial Least Squares) is adopted as algorithm of calculation. By NIPALS, T, B, and v are broken to independent elements (PLS elements), and the PLS elements are increased by 1 in turn from 1, so that eventually a model expression may be obtained with a minimal residual.

### Infrared Spectrum of a Silicon Wafer Doped with Phosphorus and Boron

Fig. 1 shows a transmission spectrum of silicon wafer containing phosphorus and boron. The peak around 1100cm<sup>-1</sup> is due to the stretching vibration of Si-O. The peak due to the stretching vibration of P-O appears at 1330cm<sup>-1</sup>. But this peak is overlapped with the band due to the stretching vibration of B-O, making simultaneous determination of phosphorus and boron difficult. Furthermore, there occurs fluctuation of the baseline depending on the samples. In such a case, it is extremely difficult to prepare a calibration curve by the multi-point calibration curve method. By applying multiple-linear regression, improvement in determination is possible but sufficient accuracy in quantitation may not be obtained. In such a case, the PLS method is effective.

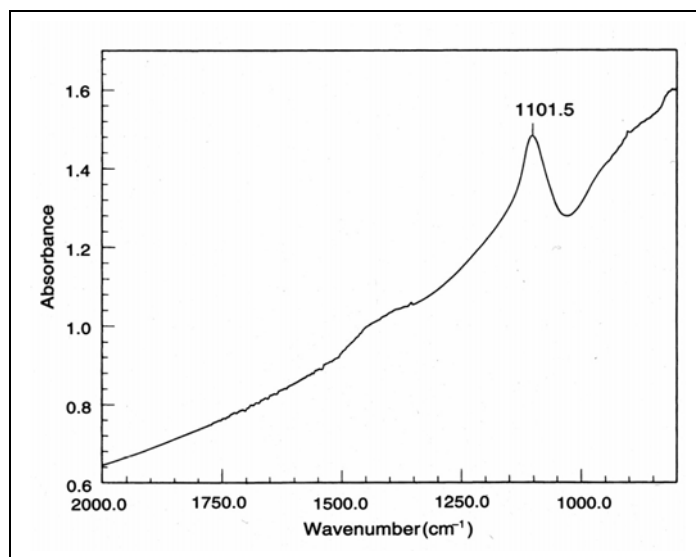


Fig.1 Infrared Spectrum of Silicon Wafer Doped with Phosphorus and Boron

Result of Quantitative Calculation

The results of quantitative calculation of phosphorus, boron, and silicon by the PLS method are shown in Table 1, Figures 2 to 4. The basic concentrations were determined by dissolving the wafer into an acid and subjecting the solution to the analysis by the ICP (Inductively Coupled Plasma Spectrometer). Favorable results were obtained for any of phosphorus, boron, and silicon samples. As an index of indicating quantitative accuracy, SEP (Standard Error of Prediction) may be given. The definition of SEP is as shown below.

$$SEP = (2(C_{pre} - C_{act})^2 / m)^{1/2}$$

Here, Cpre and Cact show predicted concentration and actual concentration respectively, and the calculation of the sum total is carried out by using all the samples. m is the number of the samples. SEP for phosphorus, boron, and silicon turned out to be 0.75, 0.78, and 0.55 wt% respectively.

Table 1 Result of Quantitative Calculation by PLSI

Concentration of Phosphorus (wt%)		Concentration of Boron (wt%)		Concentration of Silicon (wt%)		Thickness (A)	
Actual	Predicted	Actual	Predicted	Actual	Predicted	Actual	Predicted
9.83	12.57	6.09	6.29	84.08	81.65	1948	1937
14.07	13.13	5.76	6.16	80.25	81.47	1966	1951
8.19	8.04	9.07	9.15	82.74	82.54	1956	1955
9.81	9.43	8.82	8.79	81.37	81.47	1930	1957
6.24	11.21	8.43	8.59	79.47	80.56	1927	1982
7.05	7.01	2.16	1.79	81.6	81.69	1930	1891
8.76	8.13	11.59	11.56	81.36	80.71	1947	1921
10.23	9.01	11.03	11.06	80.2	80.11	2005	2013
13.58	9.41	6.07	6.07	83.7	83.88	3984	3939
16.18	13.30	5.77	5.75	80.65	81.03	3924	3950
12.41	15.67	5.79	5.84	78.03	79.34	3924	3903
9.44	11.19	5.76	6.03	81.83	82.33	1910	1931
11.72	9.44	9.31	9.12	81.25	81.28	3849	3883
14.29	12.31	8.75	8.83	79.53	78.97	3963	3993
7.99	14.26	8.4	8.43	77.31	77.50	3836	3884
10.5	8.43	12.05	11.71	79.96	79.55	3837	3809
12.33	10.55	11.63	11.32	77.87	77.88	3903	3895
10.29	11.77	10.96	11.05	76.71	76.62	3973	3911
13.96	10.21	6.18	6.14	83.52	83.60	5790	5823
16.97	14.00	5.43	5.30	80.61	80.98	5702	5665
9.64	17.38	5.53	5.48	77.5	78.06	5861	7595
12.31	9.94	9.17	9.39	81.19	80.62	5705	5701
15.65	12.84	9.16	9.17	78.53	77.73	5864	5956
8.9	15.60	8.42	8.29	75.93	75.83	5825	5884
12.82	8.71	11.98	12.13	79.11	78.38	5859	5829
15.13	12.66	11.06	11.06	76.12	76.36	5848	5836
12.1	14.72	10.42	10.54	74.45	74.73	5810	5782

Estimation of Silicon Wafer Thickness

The thickness of the wafer used in the above-mentioned analyses was not constant, but in quantitative calculation, thickness correction for making the optical path length constant was not carried out. It is comprehended by the result of quantitation that the fluctuations of the thickness of the silicon wafer may be compensated by the PLS to a certain extent. Furthermore, as is shown in Table 1 and Fig.5, this method can be applied for the prediction of the thickness itself. SEP for the thickness was 38A.

References

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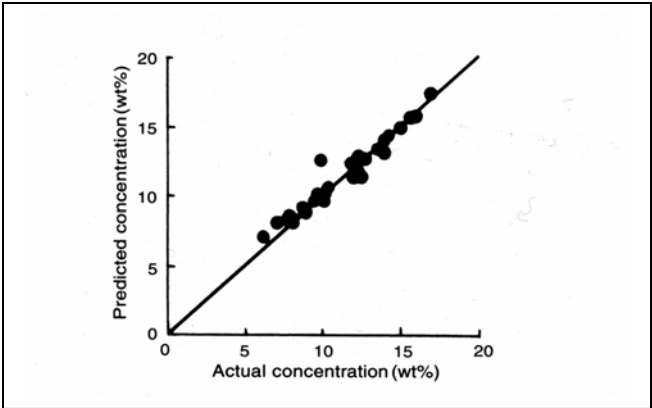


Fig.2 Relationship between Predicted and Actual Concentrations of Phosphorus

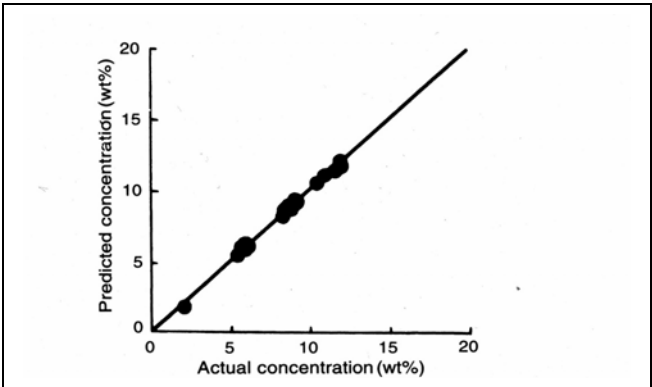


Fig.3 Relationship between Predicted and Actual Concentrations of Boron

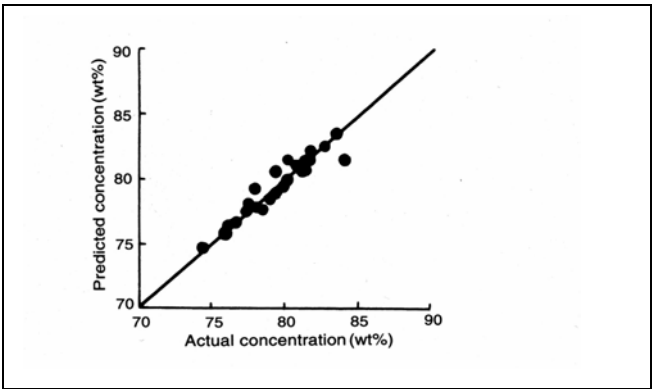


Fig.4 Relationship between Predicted and Actual Concentrations of Silicon

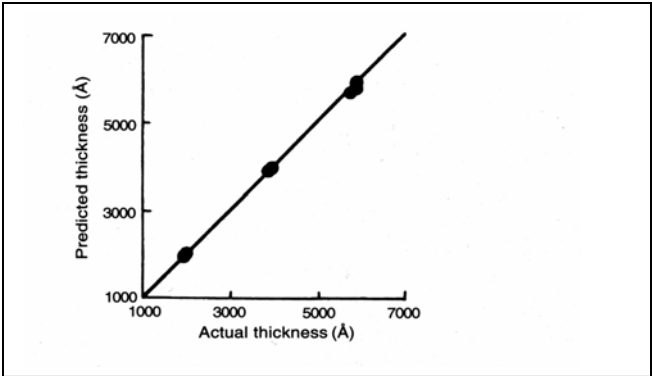


Fig.5 Relationship between Predicted and Actual Thicknesses

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