

# Growth of Co on a Silicon Oxide Surface Studied by Angle-resolved XPS

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## Theory

### Angle-resolved X-ray photoelectron spectroscopy (ARXPS)

- depth profiling of topmost layers (up to ~ 3 nm)
- non-destructive unlike SIMS and other methods

Depth profiling is not straightforward - an interative algorithm for depth profile calculations is used (Fig. 1)

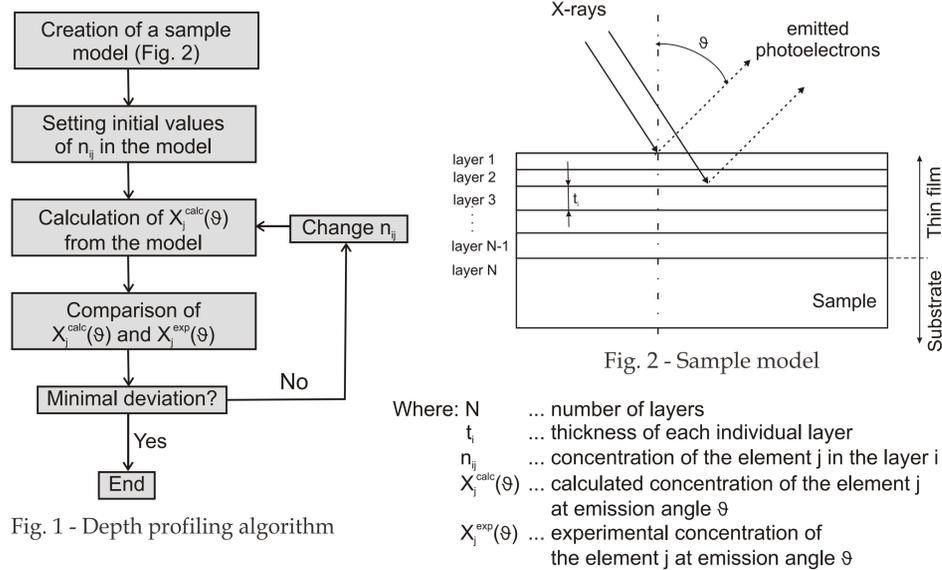


Fig. 1 - Depth profiling algorithm

### Creation of a sample model

- depth is determined by setting N and  $t_j$
- the last layer N belongs to the substrate (Fig. 2)

### Initial matrix values $n_{ij}$ can be set

- randomly
- from previous calculations
- from results of another method

### Calculation of $X_j^{calc}(\theta)$

An electron-attenuation-based method is used with elastic scattering corrections [1]

### Comparison of $X_j^{calc}(\theta)$ and $X_j^{exp}(\theta)$

- by square root deviation C

$$C = \sum_j (X_j^{calc} - X_j^{exp})^2$$

- by unsmoothness U (variant  $U_1$  and  $U_2$ ) [2]

$$U_1 = \int_0^n n^2 dz, \quad U_2 = \int_0^n n^2 \left( \frac{dn(z)}{dz} \right)^2 dz$$

- both the methods are used in a final criterion Q

$$Q = C + \alpha U$$

Where:  $\alpha$  ... regularization parameter

The way, how to calculate the realistic depth profiles is to minimize a function which calculates Q from  $n_{ij}$  and  $X_j^{exp}(\theta)$  (the closed loop in the depth profiling algorithm - Fig.1):

$n_{ij}$  is searched during the minimization.

Two methods in the Matlab environment were used in depth profiles calculations:

- genetic algorithms (GA) [3]
- "fmincon" Matlab function

Genetic algorithms are generally very powerful in finding the nearest surroundings of a global minimum, but finding an exact minimum is rather difficult. The "fmincon" function has opposite properties. Therefore, both the methods were combined as follows:

- 1) GA for selected  $\alpha$  looks for concentrations in several discrete levels (from random initial  $n_{ij}$ ).
- 2) The "fmincon" function starts from an appropriate result of GA and looks for the exact minimum in real numbers.

Described algorithm above has been successfully tested on modelled structures [4].

## Experiments

For testing the algorithm on real samples, ultra thin layers of Co on  $\text{SiO}_2$  were deposited by UHV evaporation under room temperature. Such a technique resulted in the formation of smooth uniform layers [5]. Consequently, the layers were analysed by in situ ARXPS.

### Sample No. 1

- Si (111) substrate covered by native silicon dioxide
- substrate cleaning - heating at 550 °C for 12 hours
- assumed total thickness of Co layers:

- deposition A = 0.2 nm
- deposition B = 0.6 nm
- deposition C = 1.2 nm
- deposition D = 2.0 nm
- deposition E = 2.8 nm
- deposition F = 3.9 nm

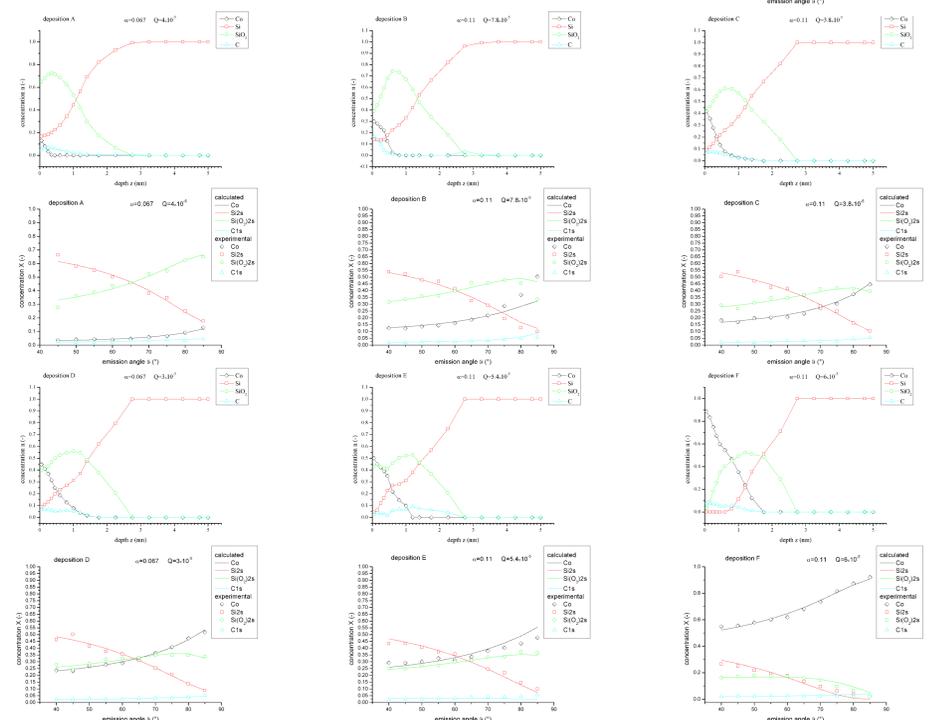
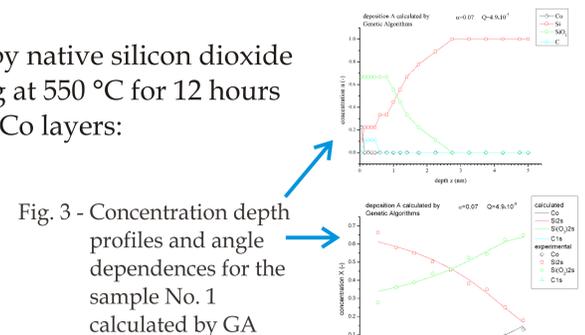


Fig. 4 - Concentration depth profiles for various layer thicknesses of the sample No. 1 calc. by "fmincon"

### Sample No. 2

- Si (100) substrate covered by thermal 45 nm thick  $\text{SiO}_2$
- substrate cleaning - heating at 600 °C for 24 hours
- each deposition (of 6) increased Co thickness by 0.1 nm

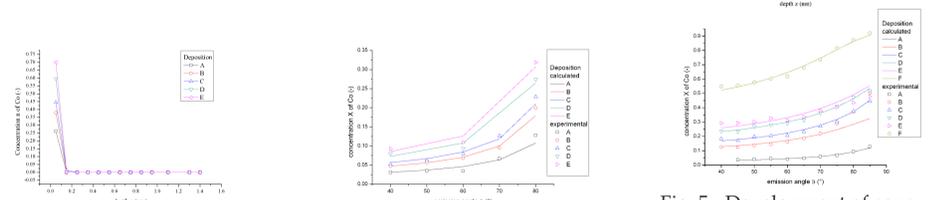


Fig. 6 - Development of concentration depth profiles and angle dependences with the layer thickness of the sample No. 2

## Conclusion

We have tested the depth profiling algorithm on real samples consisting of cobalt layers on silicon dioxide/Si substrates. The calculated depth profiles show a smaller amount of cobalt than it was determined by a thicknessmeter after the deposition. The reason is probably in less continuous cobalt layers than we assumed.

Nevertheless the amount of cobalt evidently grows with increasing time depositions, hence the algorithm mentioned above is useful for the non-destructive profiling of continuous or semi-continuous ultrathin films.

## References

- [1] M.P. Seah, I.S. Gilmore, *Surf. Interface Anal.* **2001**; 31, 835.
- [2] Z. Chanbi, R.W. Paynter, *J. Electron Spectrosc. Relat. Phenom.* **2008**; 164, 28.
- [3] C. B. Lucasius, G. Kateman, *Chemom. Intell. Lab. Syst.* **1993**; 19, 1.
- [4] J. Polčák, J. Čechal, P. Bábó, M. Urbánek, S. Průša, T. Šikola, *Surf. Interface Anal.* **2010**; 42, 649.
- [5] J. Čechal, J. Luksch, K. Koňáková, M. Urbánek, E. Brandejsová, T. Šikola, *Surf. Sci.* **2008**, 602, 2693.