

XRD analysis of tungsten thin films

I. Djerdj^a, A. M. Tonejc^a, A. Tonejc^a and N. Radić^b
^a*University of Zagreb, Faculty of Science, Dept. of Physics, Bijenička 32, P.O.Box 331, 10002 Zagreb, Croatia*
^b*Ruđer Bošković Institute, Bijenička c. 54, POBox 180, 10001, Zagreb, Croatia*

Keywords: Tungsten thin film, X-ray diffraction, Phase composition

The properties of dc-magnetron sputtered thin tungsten films depend very strongly on deposition conditions. Depending on Ar gas pressure, substrate material, substrate temperature and deposition duration, there is a different relative amount of beta- and alpha-W phase deposit. In this work tungsten thin films prepared under different conditions of working-gas pressure and deposition temperature were investigated by means of X-ray diffraction (XRD) on a Philips powder diffractometer (PW 1820) and subsequently refined by the Rietveld method using the FULLPROF program [1]. The goal of this work was to investigate the dependence of microstructure and phase composition on deposition condition. Moreover, the microstructure, size and microstrain were extracted by different methods: Rietveld method, single-line method and Warren-Averbach method. The structures were refined in the space group of α -W, $Im\bar{3}m$ and β -W, $Pm\bar{3}n$. In order to make size-strain analysis within the Rietveld method, the chosen diffraction profile function was the modified Thompson-Cox-Hastings pseudo-Voigt, with Lorentzian for size and Gaussian for microstrain. The scale factors, the background coefficients, the zero point of the detector, the lattice parameters, the Gaussian and Lorentzian halfwidth parameters were simultaneously refined. The quantitative phase composition was estimated from refined values of scale factors according to the procedure of Hill and Howard [2]. The single-line method was applied to selected well-defined non-overlapped diffraction maxima, assuming a Voigtian profile function. Last but not least, the determination of the Fourier size and microstrain coefficient using the so-called "double Voigt" method [3], which is equivalent to Warren-Averbach method, was used as an additional method for size-strain analysis. The basic requirement which must be fulfilled for the application of "double Voigt" method is the presence of two orders of reflection. This method is then applied to (200)-(400) reflections of β -W. It was found that at the deposition temperature of 293 K, on increasing the working-gas pressure, the amount of β -W phase increases. However, at low (77 K) and high (523 K) deposition temperature, on increasing the working-gas pressure, there is a sudden decrease in the amount of β -W phase at 1.4 Pa, then a further increase of working-gas pressure yields to the increase in the amount of β -W phase. The lattice parameters of alpha and beta tungsten film increase when the amount of α -W is increased, except when there is a high content of α -W (70 wt.%). The results of size-strain analysis, volume averaged grain size and r.m.s. microstrain obtained by different methods used in this work are in good agreement.

- [1] J. Rodriguez-Carvajal, FULLPROF-A program for Rietveld Refinement, Laboratoire Leon Brillouin, CEA-Saclay, France (2000).
- [2] R. J. Hill and C. J. Howard, *J. Appl. Cryst.* **20** (1987) 467-476.
- [3] D. Balzar, *J. Appl. Cryst.* **25** (1992) 559-570.