A POSSIBILITY OF APPLICATION OF MTDIL TO THE RESIDUAL STRESSES ANALYSIS
The hard coating – substrate system

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Abstract

The work demonstrates a proof of application of the modulated-temperature dilatometry (MTDIL) to the stresses investigations of the well known and commonly used hard coatings e.g. TiN, TiCN, TiAlN thin films deposited mainly on different type of tools for its higher performances.

In the PVD (physical vapour deposition) processes such kind of coatings are formed in meta stable state caused, between other, by strong stresses between coating and substrate. These stresses have an important influence on the fundamental properties of the coatings, for example, adherence to the substrate, so they are the subject of many investigations by use of different methods, mainly XRD (X-ray diffraction).

For the purpose of presentation of application of MTDIL for such kind of investigation two reference substrate materials were chosen: ARMCO steel and cemented carbide in the form suitable for dilatometric analysis covered, by actually the most conventional, TiN hard coating.

In the article the experimental results are presented, discussed and compared with simple model formed by means of finite elements method (FEM).

Keywords: hard coatings, modulated-temperature dilatometry, residual stress

Introduction

Hard coatings such as TiN, TiCN, TiAlN have been actually widely used in the tools and machine elements industry. These coatings are produced by different PVD methods, with plasma assistance, so their formation occurs in very non-equilibrium conditions, which have between others, a significant influence on the state of the stresses in the system: hard coating-substrate. The knowledge about these stresses and their control during the technological processes is very important because they determine directly the most important practical parameter of the above mentioned system mainly the adherence of the coating to the substrate.

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The total stresses occurring in such systems are called residual stresses and they are a superposition of the following components [1]:

$$\sigma=\sigma_G+\sigma_p+\sigma_{th} \quad (1)$$

where

- σ_G stresses defined as grown-in stresses resulted from the lattice misfit of the substrate and the film deposited; they are also affected by the deposition parameters, including a substrate bias voltage,
- σ_p stresses affected by phase transition occurring in the substrate while cooling following the process of deposition,
- σ_{th} thermal stresses due to the difference in the thermal expansion coefficients α of substrate and coating, and their elastic properties.

If the stresses σ_G and σ_p are subject to modification, e.g. through selection of materials and technological conditions, the thermal stresses σ_{th} shall be created if the substrate temperature is different from the temperature of the film deposition. The relation accepted by many scientists describing the changes in thermal stresses [2–4] is following:

$$\sigma_{th}=E\Delta\alpha(T_{dep}-T)/(1-\nu) \quad (2)$$

where $\Delta\alpha$ is a difference in thermal expansion coefficients between the substrate and film, T_{dep} is a temperature of film deposition, T is a temperature of the element being coated, E is Young's modulus, ν is Poisson's ratio of the coating.

Different methods for determination of the residual stresses are used, mainly XRD method and bending foil method [5–7].

Many problems are related with such kind of measurements: sophistical instrumentation, influence of the external parameters, mathematical models used for date interpretation, etc.

Additional problem exists in separation of the particular components of the total stresses.

In this article a proof of application of the modulated-temperature dilatometry (MTDIL) method [8–10], for a study of two kinds of systems: ARMCO iron substrate-TiN coating and cemented carbide substrate WC–TiN coating are presented and discussed taking into account some implications from the numerical finite elements method (FEM) [11, 12] analysis.

Experimental

As mentioned above two kinds of the samples in the form of cylinders with the length of 30 and 3 mm in diameter made from WC and ARMCO covered by the layers of TiN with the thickness of 2 μm were used. The details of the samples preparation procedure and suitable PVD's processes were the same as described in the article [13] with the bias voltage equal – 70 V and the substrate temperature 400°C.

MTDIL experiments were carried out on the thermo-analyzer of own design [14, 15]. This device permits to perform simultaneously (MTDIL), thermodifferential (MTDTA) and thermomagnetometric (MTTM) analyses at temperatures ranging from ambient temperature to 1000°C.

Direct (DIL_{DC}) and alternating (A_{DIL}) components [16, 17] of the axial deformations of the samples as a function of temperature were recorded. The following thermal processing variables were used: $\langle q \rangle$=1°C min^{-1}, A_{Ts}=10°C, ω=0.1 s^{-1}. The samples were tested at the atmosphere of laminar flow of argon at the rate of 60 mL min^{-1}.

Results and discussion

The results of the MTDIL measurements for the samples under investigations are presented in the Figs 1 and 2. More precisely, presented results concern the first investigation processes with heating of the samples, directly after removing them from the PVD coating vacuum system.

One can observe, that in the region of the temperature close to the deposition temperature T_d, changes both on the direct and alternating components of the elongation of the samples occurs. These changes are more pronounced on the A_{DIL} components. Moreover, the directions of these changes and their shapes depend on the kind of substrate materials.

One can relate different characters of the temperature dependences of the elongation of these two samples with the values of coefficients of the temperature elongation (α) of the substrates materials (α_{ARMCO}=13.7·10^{-6} K^{-1}, α_{TiN}=9.35·10^{-6} K^{-1}, α_{WC}=4.85·10^{-6} K^{-1}).

Really, the parameter Δα in Eq. (2) has different sign for ARMCO-TiN and WC-TiN samples. But this equation describes only thermal contribution to the total stresses and does not predict any nonlinear behavior of the systems under investigation.

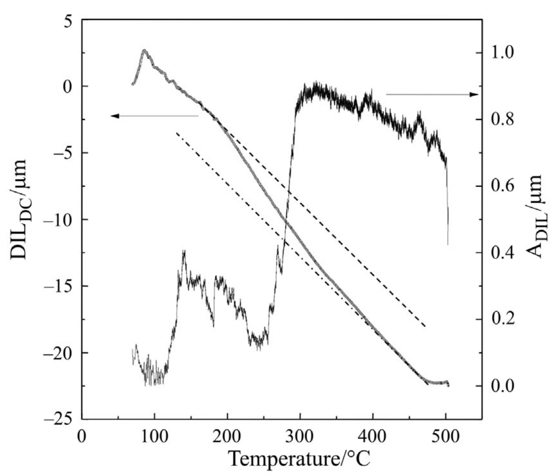

Fig. 1 Changes of the direct component (DIL_{DC}) and alternating component (A_{DIL}) of the elongation of ARMCO-TiN sample with temperature

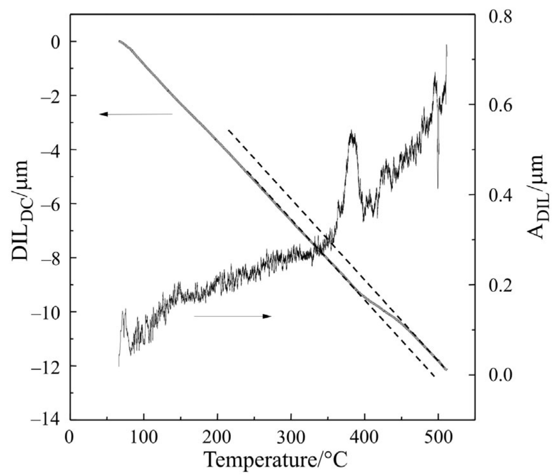

Fig. 2 Changes of the direct component (DIL_{DC}) and alternating component (A_{DIL}) of the elongation of WC-TiN sample with temperature

For the better understanding the above described results, the FEM analysis of the behavior of the both systems near T_d value with the temperature sweep (A_{TS}) [16] equal ±10 K was made.

Respecting the fact that the substrate under study is in the axial-symmetric form, the planar state of stresses and deformations in the axial section of the object has been assumed (Fig. 3).

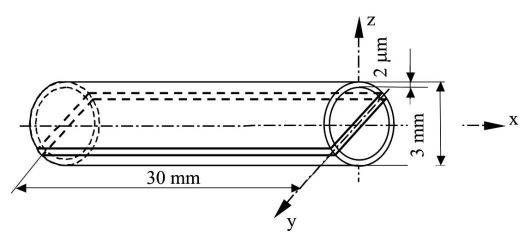

Fig. 3 Method for determination of the model for simulation calculations by FEM

The planar model composed of the substrate 15 mm×1.5 mm in dimension and the film adherent to it 2 μm in thickness was subject to investigations. The model was divided into PLANE-type planar finite elements and restrained on two axes of symmetry 0X and 0Y, which was justified regarding the measuring method in experimental investigations on the thermal expansion as function of temperature. The isotropy of quantities important for an analysis of physical properties such as the coefficients of thermal expansion α, Young's modulus E and Poisson's ratio ν of the substrate and film was also assumed. Furthermore, it follows from own experimental investigations and works [18, 19] that there is a significant influence of boundary conditions on the state of stresses in the film. Hence, the examined element is situated in the central area of the substrate section along the axis 0Y.

The following values of material constants were assumed: E_{TiN}=440 GPa, α_{TiN}=9.35·10^{-6} K^{-1}, ν_{TiN}=0.18, E_{ARMCO}=115 GPa, α_{ARMCO}=13.7·10^{-6} K^{-1}, ν_{ARMCO}=0.2, E_{WC}=650 GPa, α_{WC}=4.85·10^{-6} K^{-1}, ν_{WC}=0.24. A TiN film deposited on the substrate was 2 μm in thickness.

Figure 4 presents the values and the distribution of the stresses σ_{th} in the film and its substrate at the temperature of 20°C assuming that TiN film was deposited at the temperature of 400°C on the ARMCO substrate. A change of stress distribution near the ends of the substrates is clearly visible.

Figure 5 illustrates changes of the axial strains differences values (ΔL) in the substrate systems: ARMCO-TiN *vs*. ARMCO and WC-TiN *vs*. WC at 400°C with a programmed temperature deviation ±10°C obtained from FEM. These results have the one range lower values than of corresponding values of A_{DIL} in Figs 1 and 2.

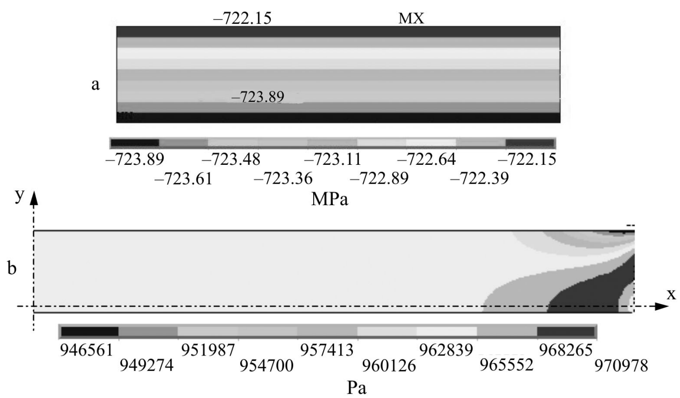

Fig. 4 Distribution of the thermal stresses σ_{th} for the FEM model of ARMCO-TiN film-substrate system. a – value and distribution of stresses σ_{th} in TiN film 2 μm in thickness at half a substrate length, b – value and distribution of stresses σ_{th} in ARMCO substrate along all the length of the substrate

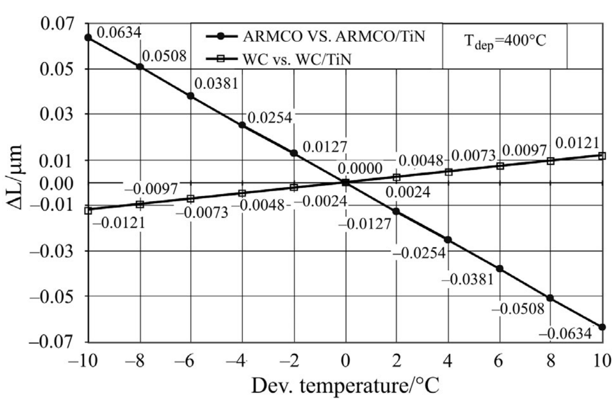

Fig. 5 Changes of the axial strains differences values ΔL in the systems ARMCO-TiN *vs*. ARMCO and WC-TiN *vs*. WC at 400°C with a programmed temperature deviation ±10°C obtained from FEM

Conclusions

The results obtained in this work indicate that MTDIL method, together with numerical modeling can be very useful for investigations of the states of the stresses in the hard coating–substrate systems.

Assuming as reported here, that during temperature investigation run any transitions in the substrate have not been occurred, these results indicates on the very important role of the σ_G component of the total residual stresses in the hard coatings.

Moreover, no presented here, on going preliminary study of the behavior of the above described system during heating–cooling cycles, indicates on the possibility of investigation the stresses relaxation phenomena. Some results, has been already published [20] in this field.

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References

1 H. Oettel, R. Wiedemann and S. Preissler, Surf. Coat. Technol., 74–75 (1995) 273.
2 V. Tomala, T. Hirsch and P. Mayr, Harterei Technische Mitteilungen, 2 (2000) 80.
3 R. C. Cammarata, J. C. Bilello, A. Lindsay, K. Sieradzki and S. M. Yalisove, MRS Bulletin, 24 (1999) 34.
4 L. Karlsson, L. Hultman, M. P. Johansson, A. Hörling and G. Ramanath, Proc. Thin Film Physics Division, Linköping University, Sweden 1999, pp. 162–189.
5 E. Zoestbergen, N. J. M. Carvalho and J. Th. M. De Hosson, Surf. Eng., 17 (2001) 29.
6 R. O. E. Vijgen and J. H. Dautzenberg, Thin Solid Films, 270 (1995) 264.
7 W. Fang, H. Tsai and Ch. Lo, Sens. Actuators, 277 (1999) 345.
8 D. M. Price, J. Therm. Anal. Cal., 64 (2001) 323.
9 P. Myśliński and P. Kamasa, J. Therm. Anal. Cal., 65 (2001) 553.
10 M. Iijima, T. Hatakeyama, K. Nakamura and H. Hatakeyama, J. Therm. Anal. Cal., 70 (2002) 807.
11 M. Kleiber, Metoda elementów skończonych w nieliniowej mechanice kontinuum, PWN, Warszawa 1985.
12 K. J. Bathe, Finite element procedures in engineering analysis, Prentice-Hall, Englewood Cliffs, NJ 1982.
13 P. Myśliński, P. Kamasa and A. Wąsik, Thermochim. Acta, 387 (2002) 131.
14 P. Myśliński, W. Precht and J. Staśkiewicz, Proc. Fourth European Symposium on Thermal Analysis and Calorimetry, Jena 1987, A 20.
15 P. Myśliński, P. Kamasa and J. Vandlik, J. Therm. Anal. Cal., 56 (1999) 233.
16 P. Myśliński, P. Kamasa and M. Pyda, 31st NATAS Conference, Albuquerque Sept. 22–24, 2003.
17 D. M. Price, Thermochim. Acta, 356–357 (2000) 23.
18 P. Myśliński, P. Kamasa and A. Wąsik, J. Therm. Anal. Cal., 65 (2001) 553.
19 B. Wendler and A. Młotkowski, Proc. 12th International Summer School Kołobrzeg'2000, 'Modern Plasma Surface Technology', Technical Univesity of Koszalin, 2000, pp. 217–229.
20 P. Myśliński, P. Kamasa and A. Wąsik, J. Therm. Anal. Cal., 64 (2001) 1201.