Dariusz Golański
Tomasz Chmielewski
Zhu Sheng

The effect of the interface profile on the residual stresses formed in thermally sprayed NiAl coatings on Al_2O_3 substrate

Wpływ kształtu granicy połączenia na naprężenia własne powstające w natryskiwanych powłokach NiAl na podłożu ceramiki Al_2O_3

Abstract

The physical preparation of a surface material to be coated by the thermal spray processing plays very important role as it affects the bonding force between the coating and substrate. When the coating material has different thermal and physical properties than the substrate the thermal residual stresses are generated in a two material system which may reach the level that promotes the coating delamination or cracking. Another factor influencing the stress state in sprayed coatings may lay in the interface profile between the coating and substrate. We may try to affect this factor by analyzing the profile and texture of the substrate surface to be coated. This way we may influence the residual stress built in a deposited coatings. The aim of this paper is to model and analyze the effect of the substrate surface profile on the residual stresses generated during cooling of thermally sprayed metallic coatings onto the ceramic substrates. The numerical computer simulation has been performed to calculate and compare the residual stress state developed in thermally sprayed metallic/ceramic system ($NiAl/Al_2O_3$). The main factor analyzed was the variation in the shape of the interface profile between the coating and substrate. The obtained results have been discussed.

Keywords: thermal residual stresses, coatings, interface profile

Streszczenie

Przygotowanie fizyczne podłoża materiału do natryskiwania termicznego odgrywa bardzo ważną role ponieważ wpływa na stopień powiązania między utworzoną na podłożu powłoką. Gdy materiał powłokowy ma różne właściwości cieplne i fizyczne w stosunku do podłoża to w takim układzie powstaje określony stan naprężeń własnych termicznych, który w zależności od wielkości i rozkładu może prowadzić do pęknięć w powłoce lub jej delaminacji od podłoża. Istotnym czynnikiem wpływającym na stan naprężeń własnych w natryskanej powłoce może być kształt linii połączenia między powłoką a podłożem. Można mieć na niego wpływ poprzez analizę kształtu czy tekstury podłoża przygotowanego do natrysku. W ten sposób możemy wpływać na stan naprężeń w natryskiwanych powłokach. Celem pracy było zbudowanie modelu obliczeniowego oraz analiza wpływu profilu linii połączenia powłoki z podłożem na rozkład naprężeń własnych termicznych powstających w fazie chłodzenia natryskanej na podłoże powłoki. Przeprowadzono obliczenia numeryczne dla układu powłoki NiAl natryskanej na podłoże ceramiki Al_2O_3. Głównym analizowanym czynnikiem był charakter profilu granicy połączenia między powłoką a podłożem. Wyniki obliczeń naprężeń własnych dla sześciu różnych profili granicy połączenia poddano analizie porównawczej oraz dyskusji otrzymanych wyników.

Słowa kluczowe: naprężenia własne termiczne, powłoka, profil linii połączenia

Dr hab. inż. Dariusz Golański, prof. PW; dr hab. inż. Tomasz Chmielewski, prof. PW – Warsaw University of Technology, Institute of Manufacturing Technologies, Department of Welding Engineering, Warsaw, Poland, **prof. Zhu Sheng Ph.D.** – National Key Laboratory for Remanufacturing, Beijing, China.

Autor korespondencyjny/Corresponding author: t.chmielewski@wip.pw.edu.pl

Introduction

The thermal spraying belongs to one of the most universal method for the deposition of coating materials used for the purpose of substrate protection against friction, erosion, corrosion or fatigue wear [1]. The application of intermetallic materials (eg. FeAl, NiAl, TiAl) for the thermal spraying is a continuously developing field of interest which results from their high strength, oxidation resistance and lower density comparing to the common nickel and iron based alloys specifically in a high temperature environment applications [2, 3].

The literature provide us with several examples of application of intermetallic materials deposited onto the metallic substrates while a very few data can be gathered on the possibility of using thermal spraying of these kind of materials on the ceramic substrates [4÷6]. Such combination of materials looks very promising as it can be used for cheap and effective method of developing protective and repair coatings as well as could be used as a fast metallization technique applied for bonding of ceramic parts [7, 8]. To achieve good bonding between the sprayed metallic coating material and the ceramic substrate it is necessary to utilize high energy deposition methods like plasma, high velocity oxyfuel spraying or detonation gun processes [9, 10].

The residual stresses in thermally sprayed coatings play a very important role as the stress level and its distribution may influence the strength of deposited layers in the production stage and service life [F, G, H, J]. The coating/substrate system composed of two materials (intermetal/ ceramic) having dissimilar thermal, physical and mechanical properties is subjected to the temperature gradient resulting from the thermal spraying procedure and parameters. This leads to the formation of a different shrinkage between bonded metallic and ceramic parts developed during cooling of deposited coatings. As a result the residual stress state will be observed within the coating and substrate material. If the stress sign, level and concentration in the coating/substrate system is unfavorable it may produce cracking around coating/ substrate interface or the coating delamination [15].

Another aspect that affects the bonding strengths of deposited coatings and also the state of thermal residual stresses is the form of preparation of substrate texture for processing. It is known that the profile of metallic substrate material for thermal spraying should be shaped in a way to produce the highest extension of the surface profile which helps to form better mechanical bonding between the coating and the substrate. On the other hand the change in the surface profile prepared for thermal spraying may affect the residual stress distribution within the coating/substrate system. By utilizing the computer numerical modeling we may investigate how the residual stresses are affected by the surface profile prepared for thermal spraying before the process begin. This way we may design the optimal surface preparation as a factor affecting the strength and durability of the coating/substrate/system.

The study reported here presents to modeling results of the effect of applying several different surface profiles of a substrate material on the thermal residual stresses generated upon cooling of a NiAl intermetallic compound deposited onto the Al_2O_3 ceramic substrate.

Residual stresses in coatings

The thermal residual stresses occurring in a flat thin coating can be roughly calculated from the formula [16]:

$$\sigma_{th} = \frac{E_C}{1-\nu_C}(\alpha_C - \alpha_S)(T_b - T_r)$$

where E is the Young's modulus of the coating, α is the thermal expansion coefficient, T_b is the temperature at the beginning of stress development, T_r is the ambient temperature and ν is the Poisson ration of the coating. The subscripts c and s denote the coating and substrate, respectively.

Equation 1 presents a simplified relationship which permits to estimate the thermal residual stresses in the elastic isotropic thin layers. There are found more detailed analytical solutions for the residual stresses estimation which take into account the thickness of coating and the substrate [17].

In a real life we have to deal with coating-substrate systems that do not apply to the above assumptions. If we look at the coatings produced by the thermal spraying processes we may see that the interface line rarely presents a straight line. As an example, the microstructure of thermally sprayed NiAl coating on the alumina ceramic substrate is shown in figure 1. We may see that the interface profile line is not a straight line, or it is rather composed of several short line connected at different angles. The external coating surface profile is even more complex making the overall thickness of the layer uneven along the interface. In case we need to account for nonlinear material behavior, temperature dependence of material properties or a complex geometry of the model samples we need to use more advanced calculation techniques that the formula presented above.

One of mostly known and used tool for this purpose is the finite element method which allows analyzing models with complex geometries under the nonlinear thermo-elastic-plastic material behavior. It is worth to remember that the numerical simulation of residual stresses by the finite element method requires also several assumptions and simplifications during model creation and analysis stage. Therefore, the results that we obtain by this method shall be treated mainly as a qualitative information that is providing us with some kind of a comparison and optimization tool applied to a group o coating/substrate models. But even such results can be very valuable as we can analyze and optimize several aspect of coating/substrate systems before we start to produce them using real manufacturing processes.

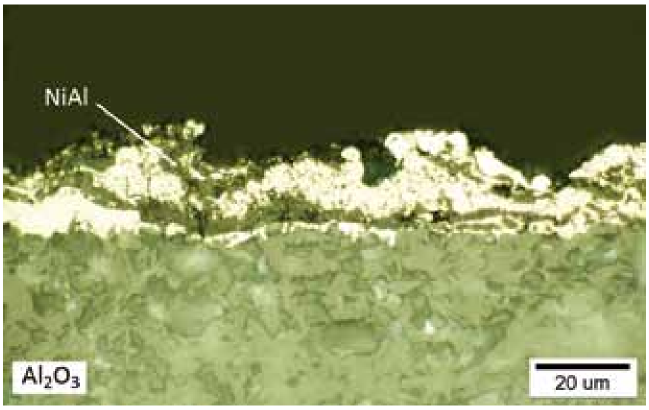

Fig. 1. The microstructure of thermally sprayed (D-Gun) NiAl coating onto the Al_2O_3 substrate

Rys. 1. Mikrostruktura powłoki NiAl natryskanej cieplnie (*D-Gun) na podłoże* Al_2O_3

Residual stress analysis in deposited coatings

The subject of analysis

The thermal residual stress analysis has been conducted for the NiAl coating models deposited onto the Al_2O_3 ceramic substrate by means of a thermal spraying process. Several NiAl/Al_2O_3 models with the variation of the coating/substrate interface profile have been prepared in order to evaluate the effect the interface profile variation on the residual stress state. The simplest model presented a 0.2 mm metal coating bonded to 1.0 mm ceramic substrate having a circular disk shape. This model represents the straight line interface profile which is utilized in the formula described by Eq. 1. Beside this basic coating/substrate system several other models have been created having different shapes of the interface profile between the NiAl coating and the Al_2O_3 substrate. All these profiles are still idealized but they represent higher degree of similarity to the real coating/substrate interface profiles.

In total six models with different profiles have built and they are presented in figure 2 together with the symbolic model description (L1-L6).

The models having higher description number presents more complicated and extended profile shape. For the purpose of the computer modeling the coating/substrate dimensions have been increased 10 times

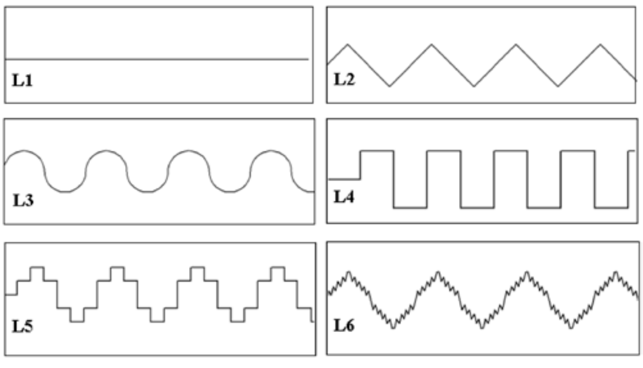

Fig. 2. The FEM models of the coating–substrate interface profiles assumed in the analysis

Rys. 2. Modele MES profilu połączenia powłoka–podłoże zastosowane w analizie

for the ease of model preparation. All models have the geometry of a disk with the 40 mm diameter, the substrate height of 10 mm and the coating height of 2 mm. The total amplitude of the surface profile was assumed to change from -0.3 mm up to 0.3 mm.

Modeling assumptions

The thermal stress analysis has been conducted using the finite element programme LUSAS v.13.8.4. The problem has been solved as a two dimensional axisymmetric model in the thermo-elastic-plastic regime with the von Mises yield criteria without material hardening. Because of model symmetry only right half of the model was used in the computations (Fig. 3).

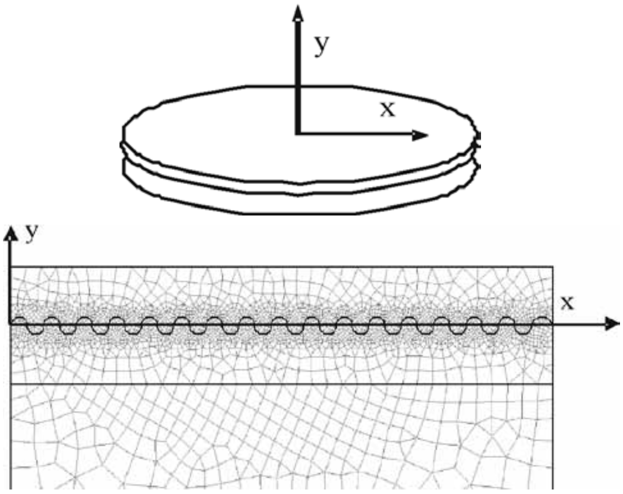

Fig. 3. Finite element mesh in one of the models (L3) of NiAl coating deposited onto the Al_2O_3 substrate

Rys.3. Siatka MES na modelu L3 powłoki NiAl na podłożu Al_2O_3

It was assumed that the residual stresses are generated upon cooling from different starting temperatures for the coating and the substrate respectively. For the thermal spraying processes the substrate temperature usually does not exceed 150÷200 °C. The temperature of the coating deposited onto the substrate is difficult to specify as it changes rapidly from the moment when the transported metallic droplets begin to adhere to the substrate. Because the analysis has a comparative meaning it was assumed that the whole deposited coating has a uniform temperature that is three times higher (600 °C) than the substrate which temperature reaches maximal value of 200 °C when the cooling starts.

The material properties used in the computations were assumed to vary with the temperature. The material data (Young modulus, Poisson ratio, thermal expansion coefficient and yield stress for the NiAl material) were taken from several literature sources [18÷22]. It is important to notice that the yield stress of NiAl intermetallic material exhibits some kind of an anomaly behavior as it drops only less than 20% (800÷650 MPa) in the range from the room temperature up to 800 °C. This is a common behavior of many intermetallic materials which is a great advantage in high temperature applications, but may result in a higher residual stresses.

Calculation results

The performed FEM analysis allowed to receive the residual stress distributions in the modeled coatings for all stress components and principal stresses. Figure 4 a, b, c show the residual stress state in NiAl/Al_2O_3 system for the model with the straight line of the coating/substrate interface profile (model L1) and the model deformation scheme (Fig. 4a) shown in the exaggerated scale. The radial stress magnitude (σx) reached 800 MPa in the NiAl coating which corresponds quite well with the stress level calculated for NiAl/Al_2O_3 system using eq. 1 from which the stress magnitude in NiAl coating was 744 MPa.

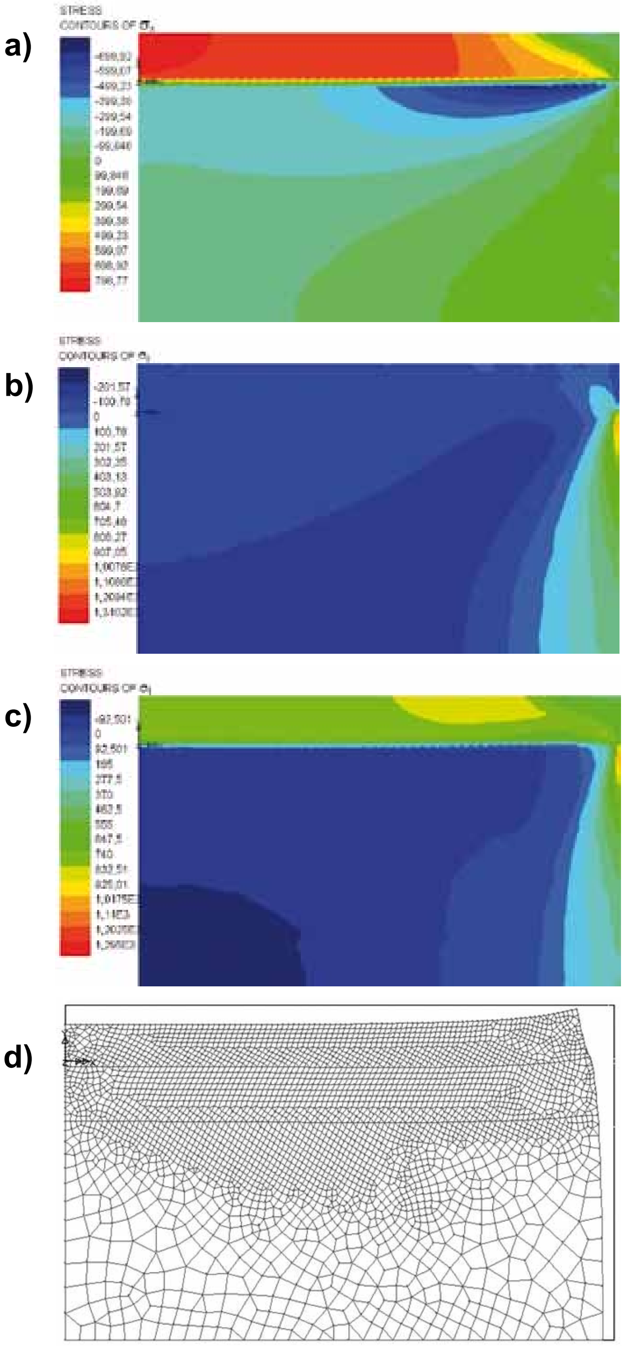

Fig. 4. Residual stress distribution in the NiAl/Al_2O_3 system (right half of the L1 model) for: a) radial σx stresses, b) axial σy stress, c) principal σ1 stress, d) model deformation

Rys. 4. Rozkład naprężeń własnych w układzie NiAl/Al_2O_3: a) promieniowe σx, b) osiowe σy, c) główne σ1, d) model odkształcenia

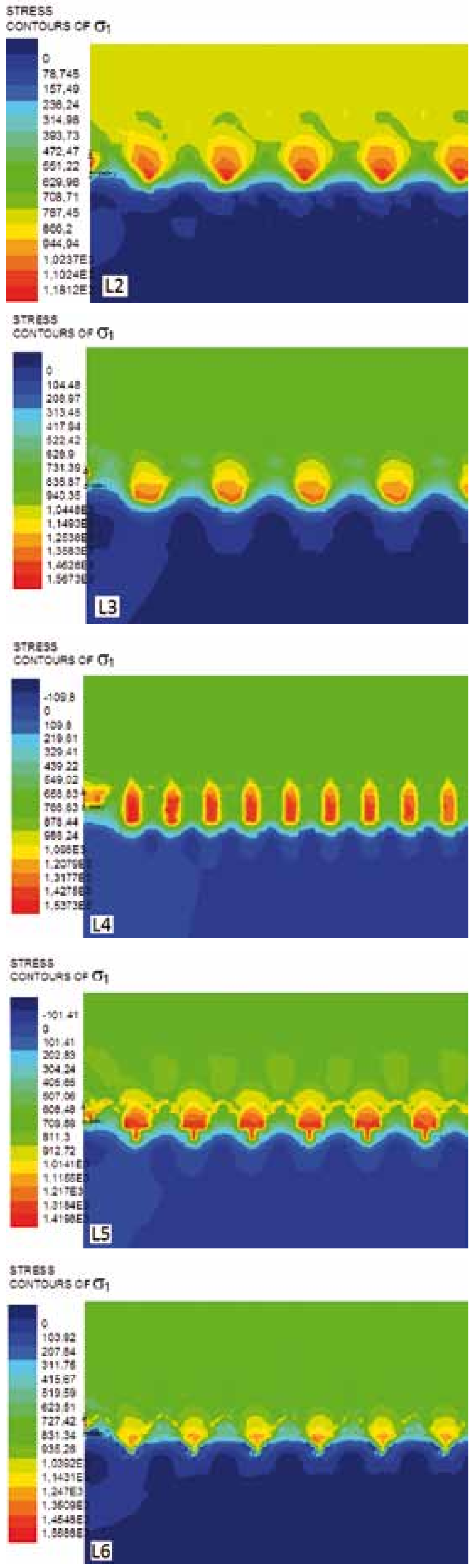

Fig. 5. Residual principal stress (σ1) distribution for the modified interface profile in the selected NiAl/Al_2O_3 models

Rys. 5. Rozkład naprężenia własnego – główne (σ1) dla profilu zmodyfikowanego połączenia w wybranym modelu NiAl/Al_2O_3

The analysis results show that the tensile radial stresses (σx) dominate within the NiAl coating and are almost uniform throughout the coating length. On the other side the ceramic substrate stays under compressive stresses in most of the regions beyond a small area near the interface line on the external edge of the model (Fig. 4b). This phenomena is well known to exist at the free edge in a two dissimilar components system and is called the stress singularity. The axial (σy) stress component has the major effect on the stress concentration in this area because the high tensile stresses may promote cracking in a ceramic substrate or pulling the coating off the substrate.

The residual stresses calculated at the room temperature for the rest models (L2-L6) having modified interface profile revealed roughly similar stress distributions comparing to the initial model (L1). For the lack of space only principal stress distributions have been shown in figure 5 for the selected models. The principal stress distribution allows to visualize both the action of tensile stresses within the coating as well as the stress concentration at the free edge in the ceramic substrate so it may be a good indicator showing dangerous stress levels both in the coating and in the ceramic substrate.

From the images in the figure 5 we may conclude that the principal stress distribution is disturbed along the whole coating/substrate interface by the repeated variations of the coating/substrate profile. It can be seen that local regions with stress 'islands' having elevated tensile stresses have been developed in a repeated form along the interface. These stresses decrease towards the external edge of the model but the stress concentration still exists in the ceramic substrate at the edge of the model. The region with the stress concentration is localized within the NiAl coating, laying near the modified interface profile as shown in the enlarged area for one of the analyzed models (Fig. 6).

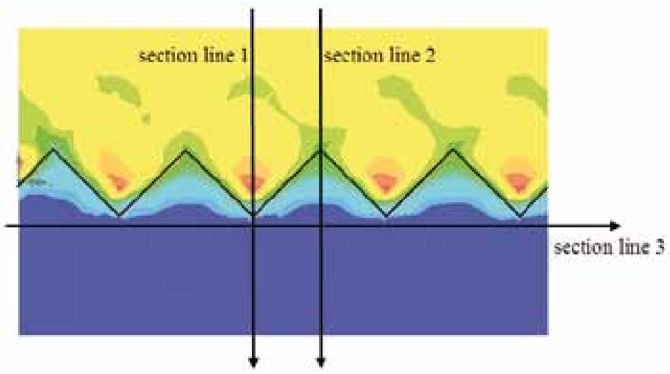

Fig. 6. The enlarged area of the stress islands within analyzed NiAl coating in the L2 model

Rys. 6. Powiększony obszar wysp koncentracji naprężeń w analizowanym modelu L2 w powłoce NiAl

To compare the stress level between calculated models two graphs of principal stress profiles across the NiAl/Al_2O_3 interface have been created (Fig. 7). One section line (1) comes through the lower part of the interface profile and the second section line comes through the upper (2) part of this profile which has been schematically drawn in figure 6.

These graphs shows that the more complex interface profile the higher the stress level is found in the coating material and also within the ceramic substrate. Specifically, the most complex L5 and L6 models present around 50% stress increase in the NiAl coating in region laying inside the profile comparing to the initial L1 model. Moreover, the residual stresses on the ceramic side within the inner part of the profile line 1 also show high stress level resulted from the cyclic shape changes on the surface of the substrate.

The tensile residual stresses within the ceramic substrate are very dangerous as it is known that ceramic materials are brittle and are 6 to 8 times weaker in tension than in compression.

The intermetallic material subjected to high tensile residual stresses may deform plastically which helps to redistribute high stress concentrations. The high yield stress of NiAl intermetalic restricts the plastic deformation to a small degree but allows to sustain its high performance at higher service temperatures.

a)

b)

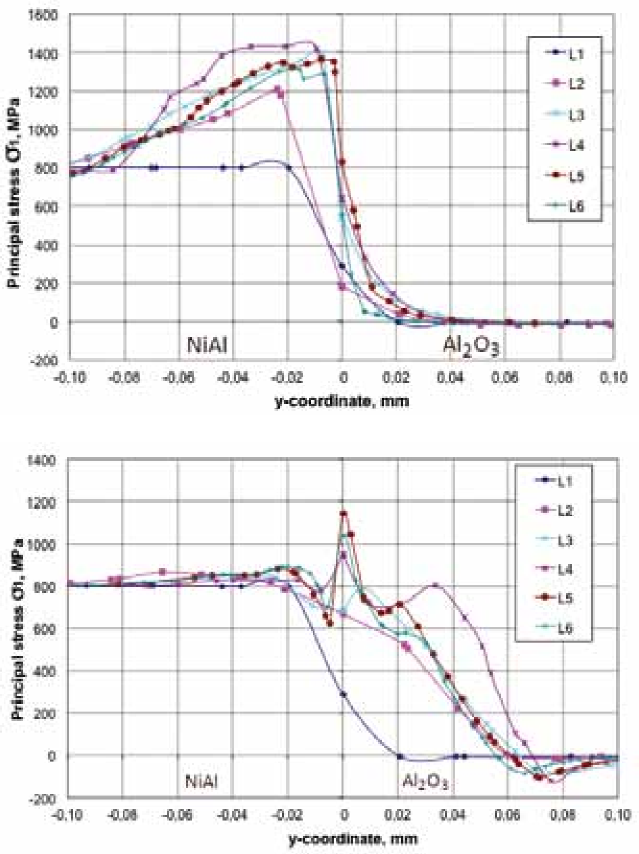

Fig. 7. The principal residual stress profiles along the section lines shown in figure 6: a) cross section line 1; b) cross section line 2

Rys. 7. Główne naprężenia własne na liniach przekroju zaznaczonych na rysunku 6: a) linia przekroju 1; b) linia przekroju 2

The changes of the principal residual stresses in the ceramic substrate towards the edge of the model are shown in figure. 8. The section line 3 from the figure 6 shows that the stress profile has been drawn just underneath the interface line of $NiAl/Al_2O_3$ system. The cyclic fluctuations of the stress level visible in this graph are due to the action of sudden changes in the interface profile.

The highest stress amplitude is observed for the L4 model and we may see that these stresses reach both tensile and compressive extreme values. The principal residual stresses in ceramic substrate reach the highest value at the edge of the model. The stress concentration visible for all models at the external edge is up to four times higher than the average tensile stress level observed far from the model edges. This is mainly due to the stress singularity formed in the FEM model as it was previously stated.

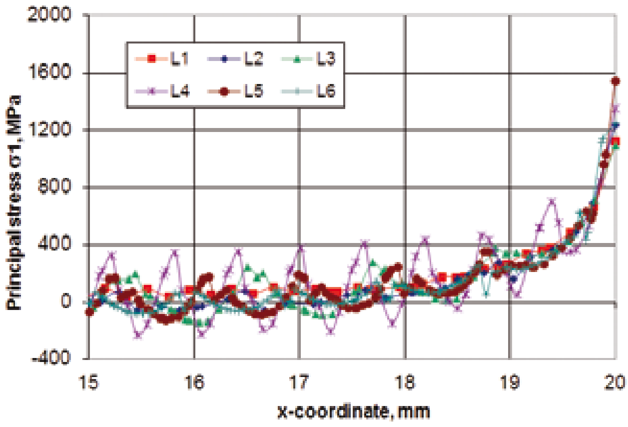

Fig. 8. Principal residual stress profiles along the interface profile at section line 3, shown in figure 6, within the ceramic substrate material for the analyzed models

Rys. 8. Główne naprężenia własne wzdłuż profili na linii przekroju 3 pokazanej na rysunku 6 w materiale ceramicznego podłoża dla analizowanych modeli

Conclusions

The computer simulation of residual stresses in NiAl coatings deposited onto the Al_2O_3 substrate demonstrated the effect of variation in the interface profile between metallic and ceramic parts on the stress distribution both in the coating and in the substrate. This analysis has comparative meaning and shows that the assumption of a straight line representing the interface between coating and substrate provides lower magnitude of tensile stress around the interface line both in the metallic and ceramic part of the model. On the other hand, the simulated complex models (L4, L5, L6) with the expanded profile of the interface line are characterized by the higher tensile stresses and cyclic stress fluctuations along the coating/substrate interface. The moderate stress changes are obtained for L2 and L3 models, still higher than that obtained in the basic L1 model. The ceramic substrate is also subjected to high tensile stress concentration at the external edge of the model which may state a potential risk of ceramic cracking or coating delamination.

The process of substrate preparation for thermal spraying by applying modification of surface profile towards the expansion of the profile line, is a widely known action used mostly in a metallic/metallic systems that helps to increase the adhesion strength between coating and substrate. In the case of ceramic substrates the advantage of such modification for the increase of a coating-substrate adhesion strength may not give favorable results as the tensile residual stresses grow up within the ceramic part. This technique could be favorable when applying other kind of metallic materials that are characterized by a lower yield stress limit comparing to the NiAl intermetallic. The higher plastic flow of the deposited material during cooling of a coating/substrate system to the ambient temperature play an important role in stress relaxation at the coating/substrate interface and may reduce the tensile stresses in ceramic substrate to the higher degree.

The analysis is a part of investigations related to the application of thermal spraying of metallic materials on the ceramic substrates to be applied as an alternative method of ceramic metallization and surface modification for high temperature applications.

The residual stresses that occurs around the interface of a metallic coating-ceramic substrate are one of the most important factors affecting the strength and durability of the whole system in the service life. The numerical computer modeling of residual stresses is one of the required initial simulation tool used for the design and selection of a coating and substrate materials combination for thermal spraying technology. The future residual stress analysis should also take into account the real surface profile of the interface line between the coating and the substrate material.

This work has been supported by the National Science Centre under the project No. NN 519652840.

References

[1] Berndt M.L., Berndt Christopher C.: Thermal spray coatings. Brookhaven National Laboratory, State University of New York, Stony Brook, 2003.
[2] Westbrook J.H., Fleischer R.L.: Structural Applications of Intermetallic Compounds. Edited by 1995, 2000 John Wiley & Sons Ltd.
[3] Trinh D., Müller M.: Aluminides. 4H1609 Functional Materials, Project Report, KTH, 2002.
[4] Chmielewski T., Golański D.: The new method of in-situ fabrication of protective coatings based on FeAl intermetallic compounds. Journal of Engineering Manufacture Part B. April 2011, 225: pp. 611-616.
[5] Gontarz G., Chmielewski T., Golański D.: Modyfikacja natryskiwanych powłok aluminiowych na stali skoncentrowanym źródłem ciepła. Przegląd Spawalnictwa Nr 12/2011, pp. 52-54.
[6] Gontarz G., Golański D., Chmielewski T.: Powłoki intermetaliczne z grupy Fe-Al wytwarzane metodami spawalniczymi. Mechanik Nr 08/09/2012, pp. 769-771.
[7] Chmielewski T., Golański D.: Wpływ tytanowej warstwy metalizacyjnej osadzonej detonacyjnie na ceramice na stan naprężeń powstających w lutowanych złączach Al_2O_3-stal. Przegląd Spawalnictwa Nr 10/2010, s. 56-60.
[8] Golański D., Chmielewski T., Gontarz G.: Badania zwilżalności ceramiki metalizowanej metodami natrysku cieplnego. Przegląd Spawalnictwa, No. 8(2013), pp. 65-69.
[9] Davis J.R.: Handbook of Thermal Spray Technology, ASM International, 2004.
[10] Chmielewski T.: Wykorzystanie energii kinetycznej tarcia i fali detonacyjnej do metalizacji ceramiki, Prace Naukowe PW. Seria Mechanika, Zeszyt 232 (2012), pp. 1-155.
[11] Chmielewski T., Golański D.: Modelowanie numeryczne naprężeń własnych w złączach Al_2O_3–Ti oraz Al_2O_3–(Ti+Al_2O_3) formowanych podczas natryskiwania detonacyjnego. Przegląd Spawalnictwa, Nr 9(2009), pp. 58–62.
[12] Chmielewski T., Golański D., Gontarz G.: Pomiar naprężeń własnych powłok metalicznych natryskiwanych termicznie. Przegląd Spawalnictwa Nr 12/2011, s. 59-64.
[13] Zimmerman J., Lindemann, Z., Golański D., Chmielewski T., Włosiński W.: Modeling residual stresses generated in Ti coatings thermally sprayed on Al_2O_3 substrates. Bulletin of the Polish Academy of Sciences – Technical Sciences, Vol. 61, No. 2, 2013, pp. 515-525.
[14] Golański D., Chmielewski T., Gontarz G., Zimmerman J., Włosiński W.: Badania naprężeń własnych w powłokach natryskiwanych metodą HVOF, Przegląd Spawalnictwa, No.11(2013), pp. 30-35.
[15] Hutchinson J.W., Evans A.G.: On the delamination of thermal barrier coatings in a thermal gradient. Surface and Coatings Technology 149 (2002), pp.179-84.
[16] Houdeau D, Steckenborn A., Zhang J-M, Kiesewetter L.: Eigenspannungen in Mikrosystemen, in Proc. Conf. „Residual Stresses", Frankfurt DGM Informationsgesellschaft, Verlag, 1992. p. 23.
[17] Araujo P., Chicot D., Staia M., Lesage J.: Residual stresses and adhesion of thermal spray coatings, Surface Engineering vol.21(2005), No. 1, 35-40.
[18] Li D., Lin D., Liu Y.: Effect of temperature on the tensile properties and dislocation structures of FeAl alloys. Materials Science and Engineering A249 (1998), 206-216.
[19] Reddy B.V., Deevi S.C.: Thermophysical properties of FeAl (Fe-40 at.%Al). Intermetallics 8 (2000), pp. 1369-1376.
[20] Schneibel J.H.: Schneibel J.H. et al, editor. Processing, Properties, and Applications of Iron Aluminides. Warrendale, PA: TMS, 1994. p. 329.
[21] Totemeier T.C., Wright R.N., Swank W. D.: FeAl and Mo-Si-B Intermetallic Coatings Prepared by Thermal Spraying. Idaho National Engineering and Environmental Laboratory. Report.
[22] Choo H., Bourke M.A., Daymond M.R.: A finite element analysis of inelastic relaxation of thermal residual stress in continuous fiber-reinforced composites. Comp. Sci. & Tech., vol. 61 (12), pp. 1757- 1772, 2001.