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Numerical simulation of displacement instabilities of surface grooves on an alumina forming alloy during thermal cycling oxidation[†]

Jun Ding[1,2], Feng-Xun Li[1] and Ki-Ju Kang[1,*]

[1]*Department of Mechanical Engineering, Chonnam National University, GwangJu, 500-757, Korea*
[2]*Department of Mechanical Engineering, Chongqing University of Technology, Chongqing, 400-050, China*

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Abstract

Displacement instability of the thermally grown oxide (TGO) is a fundamental source of failure in thermal barrier systems. In this work, a finite element analysis has been performed to analyze the displacement instability occurring at a heat resistant metal with superficial TGO subjected to thermal cycling. Lateral and in-plane growth of the TGO which happens during high temperature is simulated by means of material property change from the substrate metal to the TGO. Most of the material properties including the TGO growth are based on the results experimentally obtained in-house. Results of the finite element analyses agree well with the experimental observation, which proves the accuracy and validity of this simulation. The technique will be useful for future work on more complicated phenomena such as deformation under thermo-mechanical cycling.

Keywords: Displacement instabilities; Numerical simulation; Thermal cycling; Thermally grown oxide

1. Introduction

Thermal barrier coatings (TBCs) are widely used in modern gas turbines for propulsion and power generation. They comprise thermally insulating coatings having sufficient thickness and durability to sustain an appreciable temperature difference between the load bearing alloy and the surface [1-2]. The benefit of these coatings results from their ability to sustain high thermal gradients in the presence of adequate back-side cooling. During service, however, the formation of α-Al_2O_3 by the thermal oxidation of bond coat, joining zirconia top coat and load bearing substrate at elevated temperature induces large stresses that can cause the oxide layer to be unstable against out-of-plane displacements and even this layer to break down (Fig. 1), especially upon thermal cycling [2]. This phenomenon has attracted much attention in modern gas turbine engines, since it is often associated with the separation of zirconia top coat from the thermally grown oxide (TGO), one of the main failure mechanisms for the thermal barrier systems. The principal driving forces in the displacement instabilities of TGO are the thermal expansion misfit between TGO and the metal, the growth strains of the TGO, and the yielding or creep strength in the metal. Extensive investigations to date have been performed to

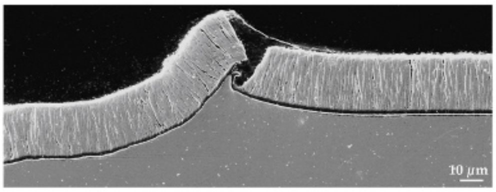

Fig. 1. TGO break-down phenomenon upon multiple thermal cycles.

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[*] Corresponding author. Tel.: +82 62 530 1668, Fax.: +82 62 530 1689
E-mail address: kjkang@chonnam.ac.kr

broaden this basic understanding of the displacement instabilities of TGO.

In the last few years, the emphasis had been placed on the deformation of TGO in the vicinity of a single dimple or a groove. Evans and Hutchinson [3] employed a numerical method for the first time to investigate the displacement instabilities for a sinusoidal undulation embedded into bond coat surface, wherein the pre-existing non-planar surface accounts for the instability. The lateral growth strain was introduced at the high temperature as a necessary condition for the occurrence of displacement instabilities, and it was found that the amplitude of undulation increases with thermal cycles. Ambrico *et al.* [4] further derived analytical results for stress distribution and plastic zone sizes, to pursue for a mechanics-based explanation for the evolution of undulations with thermal cycles. Based on an idealized model the TGO was simulated as an annular domain embedded with the elastic-plastic matrix and it was demonstrated that thermal strain, cyclic reverse yielding and oxide growth are combined together to promote the rapid evolution of displacement instability. Karlsson and Evans [5] developed a tractable numerical scheme that eliminates the restrictions of the previous models to simulate the displacement instabilities. A distinct feature was the simulation for TGO growth that involves not only lateral growth strain, as mentioned above, but also the thickening strain that contributes to the increase in the thickness of TGO at high temperature. The emphasis was on the factors that exert the key influence on the instability, such as plasticity in bond coat, growth strains in the TGO, thermal expansion misfit among TGO, bond coat and substrate, as well as stress relaxation in the TGO at high temperature. They found that the incidence of reverse yielding of bond coat upon reheating differentiates between ratcheting and shakedown. Employing such a method, Karlsson and Evans [6] probed into the sensitivity of material property, TGO thickness, and the imperfection geometry such as curvature of ratio, to displacement instability observed in an experiment with a controlled imperfection. A conclusion could be reached that, in order to realize cyclic displacements comparable in magnitude to those found experimentally, large values of oxide growth strains are required and the bond coat material must be relatively soft. Subsequently, Karlsson *et al.* [7] and He *et al.* [8] devised a spherically symmetric model to explore a fundamental understanding of the displacement instabilities and investigate the role of yielding of TGO in the instabilities.

Although considerable researches have been performed on the displacement instability induced by TGO upon thermal cycles, few works attempted to simulate the instability based on the realistic material properties such as yield stresses of TGO and substrate, and TGO growth strain at the elevated temperature due to lack of experimental data. Instead, the assumptions of constant values for material properties regardless of temperature were made for simplification. However, the environmental temperature surrounding the TBC system changes continually as thermal cycle proceeds, and the material properties depend strongly on it. Consequently, the assumption seems rather unreasonable especially for the yield strength of the substrate. Data of yield stresses of materials composing TBC systems at elevated temperature are very scarce. The review of the literature could find no proper research in which material property details for TGO, bond coat and substrate are measured in experiments.

Experimentally, Kang and his colleagues so far have done a large amount of original works. Lee and Kang [9] developed two new technologies for the first time to measure in-situ thickness of TGO formed at high temperature. One way was the LRI method (laser reflection interferometry) and the other EDM (emissivity difference method). Based on the techniques for measuring TGO thickness, two machines were devised, micro-tensile tester with displacement controlled, and micro-creep tester with load controlled. In both testers, specimens were Joule-heated through conductive grips by using a direct current power supply. Therefore, the specimens were exposed without any enclosure, which enables in-situ measurement of the specimen behaviors such as TGO thickness growth and deformation. With the aid of invented facilities, they succeeded to measure lateral growth strain and thickening rate of TGO [9-10, 12], creep and tensile properties of TGO and the substrate [9-13], and deformation near grooves on a specimen surface upon thermal and thermo-mechanical cycling [14]. These in-house experiments undoubtedly provide the precious material data input for this work and offer a good opportunity to further investigate the displacement instability exhibited by TGO.

The purpose of this work is to perform the numerical analysis of the displacement instability occurring near the surface of a heat-resistant alloy subjected to multiple thermal cycles. It is expected to give a more realistic estimation of the displacement instability by virtue of actual material properties measured from in-house experiments. The methodology for numerical analysis is also improved for simulating TGO thickening process. The comparisons between experimental and numerical results are also made to confirm the validity of the numerical method.

2. Material behaviors at high temperature

In this section, material behaviors for TGO and metal substrate are presented, which will be used in the subsequent sections. They include TGO thickness growth rate, tensile property for alumina and substrate, and lateral growth strain in TGO at high temperature of 1200℃, as well as the elastic modulus and Poisson's ratio for TGO and substrate at high temperature of 1200℃.

The material being studied for substrate of specimen was a commercially available Fecralloy heat resistant alloy with a chemical composition of Fe72.8%/Cr22%/Al5%/Y10ppm. The reason for Fe-Cr-Al-Y alloy being chosen as TGO forming material was that it can form a uniform α-Al_2O_3 scale that tends to be very flat in the absence of voids at the interface between oxide and alloy [10]. Fig. 2 shows TGO thickness growth rate where the thickness of TGO formed on the surface of Fecralloy substrate is plotted against the square root of elapsed time [9, 12]. The curve corresponds to the specimen used in the groove deformation test (discussed later) upon thermal cycling. Note that for the curve, as the TGO thickness increases, the thickness growth rate decreases more rapidly than a typical parabolic law, which indicates that the use of constant thickening growth strain appearing in prior assessments was unreasonable [1, 3, 5-8].

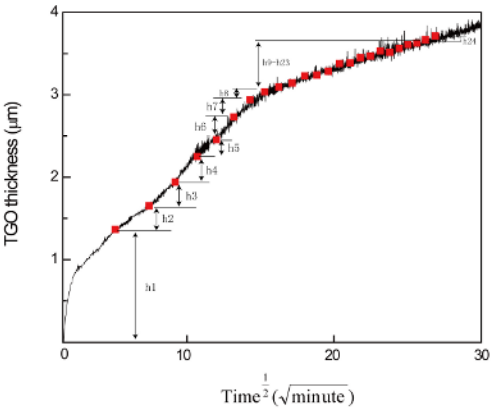

Fig. 2. The variation of the thickness of TGO with the square root of the oxidation time. The values of h1~h24 are the thickness of TGO formed in each thermal cycle.

Fig. 3(a) to 3(b) [11] provides the data of tensile properties for substrate and TGO at high temperature, respectively. Fig. 3(a) shows the stress-strain curve for the Fecralloy substrate which was tested at high temperature in argon environment. It indicates that the yield stress of substrate at elevated temperature is about 7.6 MPa. Fig. 3(b) gives the stress-strain relation for TGO which was formed on the surface of substrate. The curves for three TGO thicknesses, 1μm, 2 μm and 3 μm, are illustrated. The data for yield strength of TGO appears somewhat scattered after the initial point for different thickness; however, the stress levels at which yielding commences are consistent for three cases, indicating that the yield stress value for TGO at high temperature is about 70 MPa.

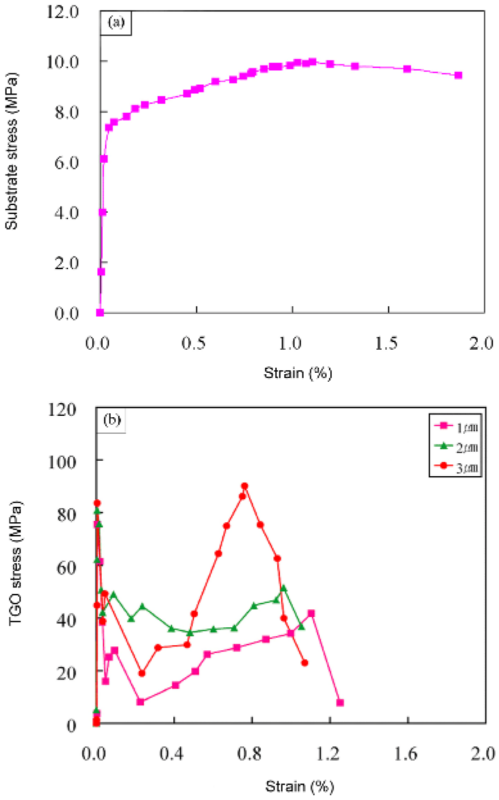

Fig. 3. The tensile property for substrate and TGO at high temperature of 1200℃. (a) The stress-strain relation of substrate in argon environment, (b) The stress-strain relation for TGO with different thickness.

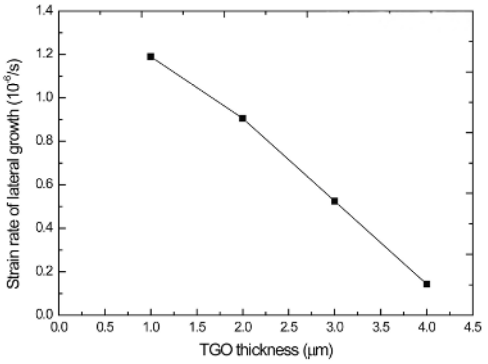

Fig. 4. The strain rate of lateral growth versus TGO thickness.

Fig. 4 shows the lateral growth strain rate of TGO which was formed within the interface between columnar grain boundaries of existing TGO at high temperature. The growth strain rate decreases rapidly as TGO thickness increases. The value of strain rate for TGO thickness of 2 μm is lower than that for TGO thickness of 1 μm. When TGO thickness exceeds 2 μm, the decreasing rate of lateral growth strain behaves almost in a linear way as TGO thick ens, indicating that TGO thickening inhibits it from lengthening. The reason for such a phenomenon is that a thicker TGO means a much longer path than a thinner one; therefore, it needs more ions and more time for chemical reaction to form new alumina along the boundaries, which results in a lower lateral growth strain rate with TGO thickness increasing [10].

As for the elastic modulus and Poisson's ratio of TGO and substrate, these values usually change with the temperature in reality. However, due to the technical difficulty in experimentally measuring the variation in magnitude with temperature and their relatively less importance in displacement instability of TGO, they are assumed to be constant regardless of temperature. According to the references [1-2, 5-8], the assumption will not influence the essence of the work.

3. The finite element procedure

When oxidation occurs, Al ions coming from the substrate react chemically with O anions ingressing from air to form alumina upon thermal cycles. Fig. 5 illustrates some of new TGO resides between the internal grain boundaries causing it to elongate, while most of TGO prefers to the sites between TGO and substrate, which results in TGO thickening [1-6, 10].

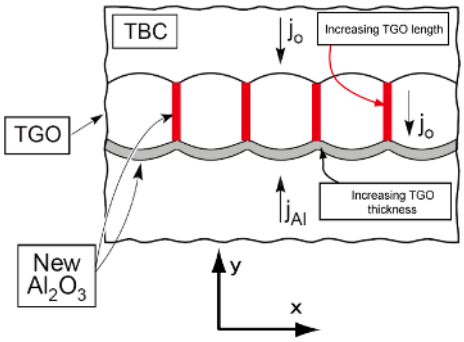

Fig. 5. The oxidation mechanism happening at high temperature.

The TGO formation at elevated temperature was simulated by the two components in the previous studies [2-8], namely, lateral growth strain and thickening growth strain. The methodology used in these works can simulate displacement instability of TGO based simply on an ideal assumption of material properties and easily confined by the limitation that total TGO thickness is much less than the initial TGO thickness. Consequently, a different strategy for simulation is required in this work in accordance with the actual material characteristics.

3.1 TGO lateral growth

TGO lateral growth can significantly influence the displacement instabilities, such as producing compressive stresses in TGO that is essential to the instability [7] and contributing to the creep deformation of TGO under tensile stresses at high temperatures [10].

According to Fig. 4, it is apparent that the lateral growth strain varies with TGO thickness. In contrast to other works [1, 4-8], the lateral growth strain of TGO at high temperature exhibits the strong dependence on the thickness of TGO, with the value of lateral growth strain rate decreasing rapidly as TGO thickens. For incorporating this trend into a finite element scheme to simulate reality, the process of TGO growth can be divided into four parts in terms of TGO thickness, that is, TGO thickness from 0 to 4μm with an interval of 1 μm. Consequently, the lateral growth strain value corresponding to each thickness part can be obtained, and thus four different lateral growth strains will be used in this work during the period of TGO growth in which the final TGO thickness after 24 thermal cycles amounts to around 4 μm.

With regard to the finite element procedure presented here, the implementation of lateral growth strain is as follows. Since the lateral growth of TGO occurs during oxidation phase at each thermal cycle, the lateral growth strain can be applied only at high temperature as a stress-free strain [1] in accordance with *uexpan*, which is a user subroutine used to define incremental thermal strain by user code in ABAQUS. Upon cooling and reheating phases, no lateral growth strain is imposed. Prior to the treatment on lateral growth, the thickness of TGO which was formed during each thermal cycle can be in advance determined from Fig. 2. It will be discussed in next section. As soon as the TGO thickness for each thermal cycle has been obtained, we then divide 24 thermal cycles into four sections according to the thickness of TGO. For instance, section 1 contains a few thermal cycles during which TGO forms from 0 to 1μm of thickness, section 2 TGO from 1 to 2 μm, section 3 TGO from 2 to 3 μm, and section 4 TGO from 3 to 4 μm. Thus, the correspondence between lateral growth strains and thermal cycle sections can be given with ease, such as section 1 corresponding to one lateral growth strain, section 2 to another lateral growth strain, and so on. Consequently, when dealing with ABAQUS input file, the different lateral growth strains can be applied within its corresponding thermal cycles to realize the dependence on TGO thickness. It can be implemented by modifying a corresponding variable appearing in ABAQUS input file with the aid of a user subroutine *uexpan.*

3.2 TGO thickening growth

As indicated previously, the simulation for TGO thickening in previous works [2-8] shows the following features: (a) using a constant value of thickening growth strain, and (b) making only a layer of elements thicken. An initial TGO layer of a given thickness was firstly taken into account for preoxidation of substrate. Then, the thin layer was uniformly meshed into a few layers of elements. TGO thickening was modeled to occur only in the lowest layer of initial TGO and a thickening strain taken as a constant for every thermal cycle was added in the layer of elements. Thus, the method was typically constrained by the limitation of large TGO thickness. It is available only for the case of final TGO thickness which is less than the initial thickness. However, the experimental result (Fig. 3) indicates that final TGO thickness after multiple thermal cycles generally attains 3 μm or more, which far exceeds the initial TGO thickness. Hence, the method failed to reflect actual thickening of TGO and could not simulate reality for large thickness of TGO.

In pursuit of eliminating the restriction from previous method, a distinct way will be employed to deal with TGO thickening which should focus on the actual TGO thickness rather than on the thickening growth strain. The relation between TGO thickness and the square root of oxidation time is already illustrated in Fig. 2, and the oxidation time at TGO growth could be readily achieved for each cycle. Therefore, it is easy to obtain the exact thickness of TGO which was formed at each thermal cycle.

For the sake of convenience of expression, h1, h2 and till h24 are employed to denote the thickness of TGO formed in the first cycle, the second cycle and the 24th cycle, respectively. When constructing a finite element model, we should firstly model Fecralloy substrate, secondly model initial TGO part and place it on the top of substrate to account for preoxidation, and then divide Fecralloy substrate into two parts. The top one represents TGO which was formed during all 24 thermal cycles with its thickness equaling to the value obtained in experiment. The dimension is measured downward from the interface between initial TGO and substrate. As such, the model consists of three parts, initial TGO part, TGO thickening part, and substrate part. The TGO thickening part is different in essence from the initial TGO one which is located on the top of substrate. The TGO thickening part means that alumina which was formed from Fecralloy substrate by chemical reaction while initial TGO represents preoxidation prior to onset of thermal cycle. Next we mesh the TGO thickening part into 24 layers of elements with each layer representing a thickness of TGO which was formed in one thermal cycle. Namely, starting from the topside of TGO part, it successively represents the TGO formed in the first cycle, the second cycle and till the 24th cycle, respectively.

3.3 Material property change

Since no new alumina forms in advance prior to thermal cycle oxidation, the process of TGO growth will be simulated here by a method of material property change which can model the successive formation of TGO from substrate material. It can be materialized by using the capability of user subroutine *usdfld*, which can be used to redefine the field variable at a material point by user code in ABAQUS software.

Upon completing construction of the finite element model in a manner discussed above, all of elements but the initial TGO part are assigned as substrate material property before executing analysis. The initial TGO part is assigned as TGO material property. Because at this time thermal cycling oxidation has not yet happened it implies an initial state prior to onset of cyclic oxidation. A newly introduced variable, SDV (solution dependent variable) in ABAQUS software appearing in user subroutine *usdfld,* can be employed to control over the material property change between TGO and substrate property. The value for SDV determines when and how the property change happens, that is, when the value equals to zero it indicates that the elements of TGO part is not alumina but still made of substrate. Meanwhile, when the value equals to one it means that the elements occupying TGO thickening part have already changed into TGO from substrate and the value ranging from 0 to 1 means that substrate is transferring into TGO increasingly. Based on such an idea, the subsequent code appearing in *usdfld* aims at how to change the value of SDV to realize the simulation of oxidation.

In the first thermal cycle, the uppermost layer of elements in TGO thickening part, equivalently, closest in location to the initial TGO part, changes its material property from substrate to TGO through controlling over the value of SDV in user subroutine, making it vary in magnitude from 0 to 1 and indicating the formation of new alumina. And in subsequent thermal cycles, the value of SDV for this layer element keeps at 1 all long until the end of a complete thermal cycle history, implicating that it has already totally changed into TGO material since the second thermal cycle. For the second thermal cycle, the layer of elements below the just already transferred one is also changed from substrate material property to TGO in a same way. Analogously, such transfer needs repeat 24 times for a complete simulation until 24 layers of TGO are entirely formed.

4. Case study

4.1 Description of specimen

The specimen was acquired in the form of cold-rolled sheets having thickness of ~500 μm. The sheets were then cut into foils with lateral dimensions ~5 mm×50 mm. Thereafter, they were mechanically ground and polished on both sides to 3 μm finishes. Two different orientation groups, one along the horizontal direction and the other vertical direction, were milled into one side of specimen. Each group consists of two grooves with similar dimension of 20±5 μm deep and around 160 μm wide. The 3-D surface profile for a typical groove and specimen configuration are illustrated as Fig. 6.

The specimen subsequently experienced 24 thermal cycles. The load sequence for experiment in the thermal cycles begins at a stress-free state, and for one typical cycle it comprises a 10 minutes ramp down to ambient from high temperature, a 10 minutes ramp up to high temperature from ambient, and a 30 minutes holding time at elevated temperature, as shown in Fig. 7. After the prescribed oxidation, the specimens were cut along the groove sections, polished again and examined by scanning electron microscopy. A typical cross section of groove is shown in Fig. 8. The white dotted line represents the initial shape prior to

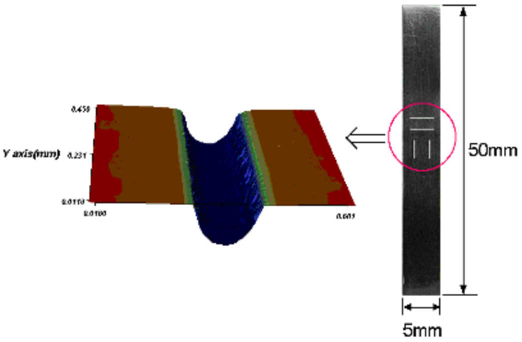

Fig. 6. The 3-D profile of the surface groove and the specimen configuration.

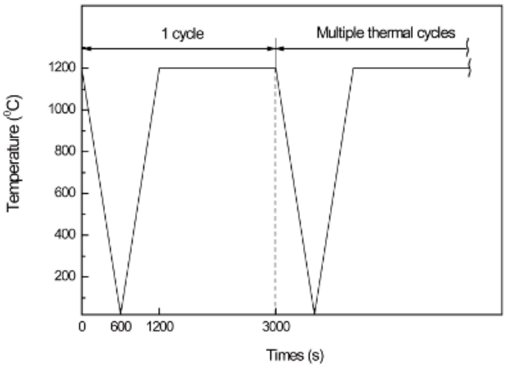

Fig. 7. The temperature loading history for one typical thermal cycle.

experiment. The final deformed shape profile after oxidation is superposed onto the original one and substantial deformations were markedly observed.

4.2 Geometry and model description

The geometry model being studied simulates the cross section which would be obtained by cutting the specimen (Fig. 6) along the horizontal centerline to expose a shape of the vertical grooves. One of the grooves was chosen from the cross section (Fig. 8). Considering that the dimension of the groove is relatively small compared to the width of specimen, the model simulates the vicinity of one side of the groove. The model dimension and the mesh representation are presented in Fig. 9. In sharp contrast with previously used typical structure [1, 3-8], this model consists only of two layers, TGO and substrate, because the substrate here plays dual roles, acting as substrate and TGO forming material to provide Al element as the source for chemical interaction to create alumina.

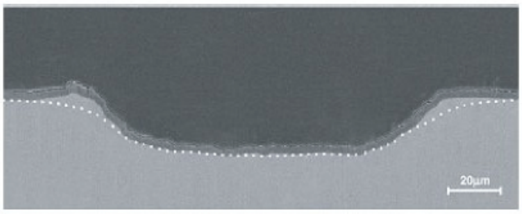

Fig. 8. The typical cross section of the specimen after twenty-four thermal oxidation cycles indicating the displacement instability of TGO near the groove.

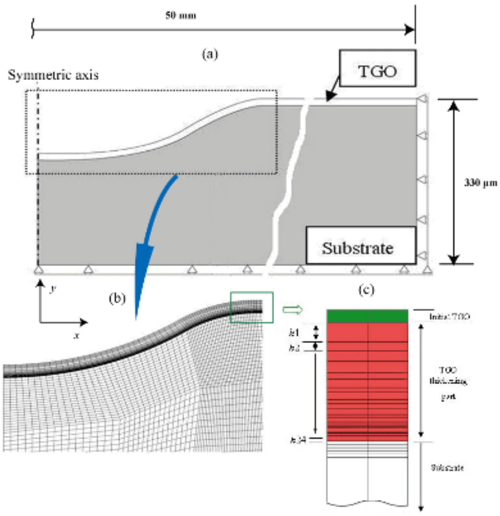

Fig. 9. The geometry model and mesh representation of the specimen. (a) the geometry model and the boundary condition, (b) the detail mesh near the groove, (c) the mesh representation used for the material property change to simulate TGO formation.

The finite element model consists of 9936 quadrilateral, first-order generalized plane strain elements, CPEG4 in ABAQUS, with the number of the elements determined by the mesh dependency check of computation. Because of the geometrical symmetry, half model is taken into account. The symmetric boundary condition is imposed on the side at $x=0$. The nodes on the right side are allowed to move in the x direction, but the movement is constrained such that all of these nodes have the same displacements. Analogously, the same method is applied for the nodes at the bottom side, while keeping the same displacements in y direction to avoid the bending deformation occurring in the period of cooling and reheating induced by thermal expansion. To avoid the rigid displacement of the overall system in y direction, any one node in the model is chosen to fix the displacement in y direction.

The material properties used in the simulation are summarized in Table 1. The dependence of elastic modulus and Poisson's ratio on temperature is ignored, and constant values for them are used for calculation. As shown in Fig. 10, the yield stresses of TGO and substrate are given as functions of temperature. For the Fecralloy substrate, the yield stress up to temperature T_1 (taken as 300℃ in calculations) is 200 MPa, and at temperature above T_2 (900℃ in calculations), the yield strength is 7.6 MPa (Fig. 3(a)). In the intermediate temperature, the yield stress is assumed linearly decreasing with temperature. With regard to TGO, during one typical thermal cycling, TGO is assumed to be elastic-perfectly plastic material behavior [1, 3, 5-8], that is, the TGO yields at elevated temperature (taken as 1200℃ in this analysis) when induced stress exceeds $\sigma_Y^{tgo}=70$ MPa (Fig. 3(b)), while upon cooling and reheating it behaves elastically.

Table 1. Material properties used in numerical simulation.

	TGO	Substrate
Young's modulus (GPa)	390	140
Poisson's ratio	0.2	0.3
Thermal expansion Coefficient (ppm/^{0}C)	8.3	11.3

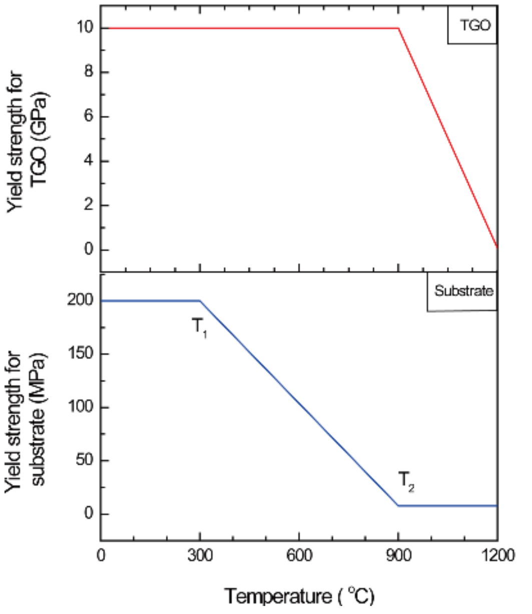

Fig. 10. The yield strength for TGO and substrate. The value of yield strength of TGO at room temperature and the variation of the yield strength of TGO and substrate depending on temperature are cited from the reference [1].

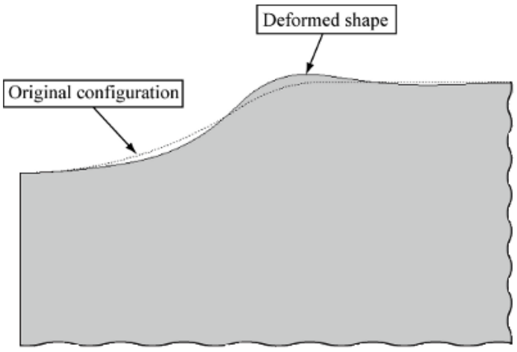

Fig. 11. The final deformation of specimen after twenty-four thermal cycles showing the displacement instability occurring near the groove.

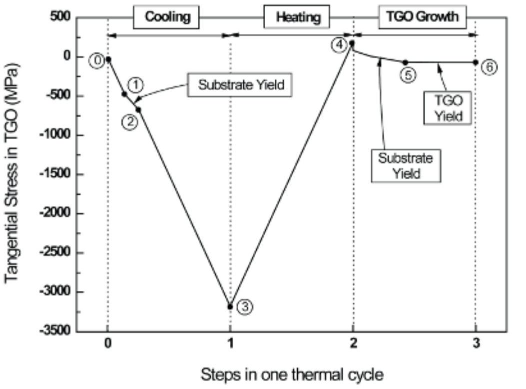

Fig. 12. The variation of tangential stress in the initial TGO layer with the steps in one typical thermal cycle.

5. Results and discussions

A simulation was performed upon 24 thermal cycles with the above-mentioned material properties, wherein the initial TGO is very thin with the thickness of 0.1 μm. Fig. 11 shows the final deformation of the model after 24 thermal cycles which illustrates the displacement instability of TGO exhibited by the groove embedded on the surface of the substrate.

The representative cross-section of the grooves aligned in horizontal orientation (shown in Fig. 6) on the surface of specimen is experimentally illustrated in Fig. 8. Both numerical and experimental results show that the periphery displaces upward while the base of groove displaces downward, resulting in a substantial increase in the amplitude of the predefined groove as the thermal cycle continues. It is apparent that the larger upward displacement occurs at the periphery and smaller at the base of the groove, in agreement with [15] wherein for the convex configuration TGO expands radially while TGO contracts radially for the concave case.

For the sake of elucidating the system response upon thermal cycles and exploring the deformation mechanism, one typical element in the initial TGO layer, which is next to the interface between the initial TGO and TGO thickening part, has been investigated for the first thermal cycle. Fig. 12 shows its tangential stress variation with the steps in one thermal cycle. As mentioned before, one complete thermal cycle consists of three steps, cooling, reheating and TGO growth. Suppose that the first thermal cycle begins at the peak temperature (position 0), about 1200℃ in this work. Firstly, since the temperature cools down gradually, a compressive stress develops in the TGO and builds up rapidly due to the thermal expansion misfit between TGO and substrate. As the surrounding temperature is high, the substrate is relatively soft (as illustrated in Fig. 10) and starts to yield (position 1), enhancing the plastic deformation in substrate. With the temperature cooling down to about 900℃, the substrate becomes stiff again because of its dependence of material behavior on the temperature. Consequently, the yielding of substrate ceases at this time (position 2) and behaves elastically leading to the rapid increase in compressive stress of TGO and attaining a considerable value. From position 3, the system is subjected to reheating from the ambient temperature; the heating is equivalent in essence to the unloading of the system so that the compressive stress decreases and alleviates the compressive state in the TGO. At TGO growth phase, the compressive stress in TGO increases rapidly because of the application of lateral growth strain and the newly created formation of TGO by transferring material property from substrate. The compressive stress firstly causes the underlying substrate to yield till the position 5 by applying a pressure [7]. With the compressive stress continuing to build up, it attains the yielding strength of TGO and finally makes TGO itself yield until the onset of the next new thermal cycle (position 6). The amplitude change in surface groove as a demonstration of displacement instability is just a result of the plastic deformation of substrate occurring in the thermal cycle. Fig. 13 shows the final amplitude change of the groove with the number of thermal cycles. It is accumulated cycle by cycle resulting consequently in a drastic increase in amplitude of groove embedded in the surface of substrate.

With the purpose of indicating the validity of TGO formation transferring from substrate material property, two typical elements, one in initial TGO layer and the other in the first layer of TGO thickening part, are chosen to show the variation of von Mises stress with the number of thermal cycles, as illustrated in Fig. 14. The first layer of TGO thickening part is expected to change into TGO material property from the substrate in the first thermal cycle, and retain TGO material property until the end of thermal cycles. It is evident from the figure that in the first thermal cycle the von Mises stress distribution differs in the two elements, and the stress in the first layer of TGO thickening part is much smaller than that for the initial TGO part because at the moment the overall TGO thickening part consists of only substrate, much softer than TGO. However, from the second thermal cycle, the von Mises stress curves for two elements coincide completely with each other, implying that this layer of substrate material has already transformed into TGO.

The experimental result for the final deformation of specimen subjected to 24 thermal cycles has been superimposed on the numerical result, which shows a reasonable agreement (Fig. 15) and proves the validity and the accuracy for this work. Upon thermal cycles, the protruding portions at the periphery of

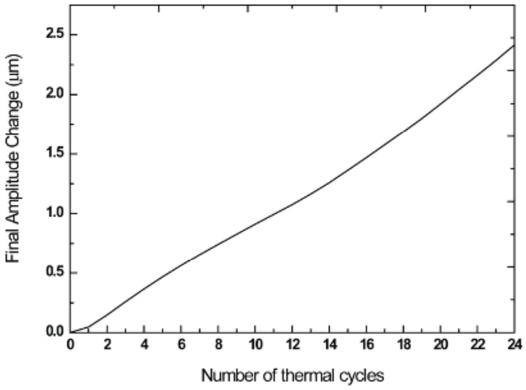

Fig. 13. The final amplitude change in the surface groove as the number of thermal cycles.

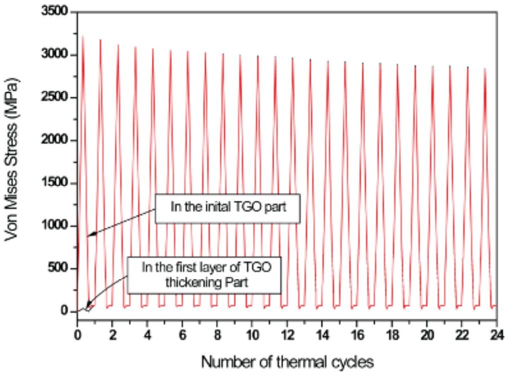

Fig. 14. The variation of von Mises stress in the initial TGO part and in the first layer of TGO thickening part with the thermal cycles, showing the validity of the material property change to model TGO formation.

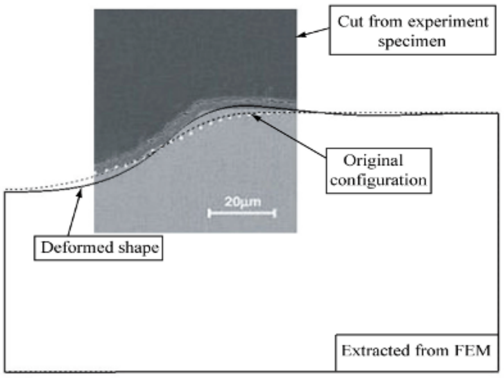

Fig. 15. The comparison between the results from the numerical simulation and the experiment observation after twenty-four thermal cycles showing a reasonable agreement in between.

groove become sharper and sharper, equivalently, the curvature radius smaller and smaller at this location, which corresponds to the observation of the experiment. For the deformation at the base of the groove, the estimated downward displacement is somewhat larger than that observed in the experiment. The slight discrepancy between them is attributed to the different groove shape. To be specific, the base of groove is much shorter in the model than in the specimen. The difference can be identified by comparing Fig. 8 and Fig. 9. The length of the groove base of the model is almost zero, while that of the specimen is more than 60 micrometers which is three times as long as the initial depth of the groove. Consequently, the upward displacement at the periphery of groove can cause a deeper downward deformation at the base of groove for the model due to the conservation of volume.

Additionally, one may argue that the assumption of the constant CTE for TGO and the substrate could make error in the result because materials, particularly ceramics like TGO, have a wide variation of CTE over a large range of temperature. To address this issue, a recalculation with CTE varying with temperature was performed. The comparison of results between with and without considering the temperature-dependent CTE of TGO and substrate, however, shows almost no difference in between suggesting that the variation of CTE with the temperature has an extremely slight effect in the present analysis. Accordingly, the finite element results with constant values of the CTE for TGO and substrate can be acceptable.

As stated previously, the advantage of this work over the previous one by Evans et al. [1, 5, 8] is that this work has the capacity of simulating the displacement instability for the larger thickness of TGO. For this purpose, a comparative study between two methods is presented by two individual finite element analyses. The material properties used in both analyses such as elastic modulus, Poisson's ratio and yield stress for substrate and TGO are obtained from an in-house experiment (same as the previous analysis) and are taken as the same values for two analyses for the convenience of comparison. The method dealing with the TGO thickening differs for two methods in that the present method focuses on the actual thickness of TGO formed in each thermal cycle, while the previous one on the TGO thickening strain. To assure the same thickness of TGO formed in each thermal cycle for two methods, the initial TGO thickness of the model is assumed as 1.0 μm and the nominal increased TGO thickness for two methods as 1.2 μm during 24 thermal cycles such that the increased TGO thickness in each thermal cycle for both methods is 0.05 μm. Note that the determination of the nominal increased TGO thickness for the previous method is from [1]. For the present method, the equal TGO thickness is assumed for each thermal cycle although it seems inconsistent compared to the description stated in the previous sections. In probing the difference of two methods, we believe that this assumption made here cannot influence the essence.

The plot of variation of final amplitude change of groove against the number of thermal cycles for two methods is illustrated in Fig. 16. It is apparent that significant differences are observed for the two methods. In the first few thermal cycles, the predicted values for amplitude change are very similar for two different methods. However, as the number of thermal cycle increases, it has been found that the error between the two methods accumulates after the first 8 thermal cycles with increasingly appreciable discrepancies. The value predicted by the previous method is markedly observed much bigger than by the present method. Furthermore, when the number of thermal cycle exceeds 20, no result data is shown for the previous method since the analysis was exceptionally terminated with too much nonlinearity occurring in the calculation. However, the present method can still work for the subsequent thermal cycles and show continuous increase in the displacement providing the reasonable results. This can be explained as follows. In the previous method, the thickening of TGO formed in thermal cycles is simulated by a strain like

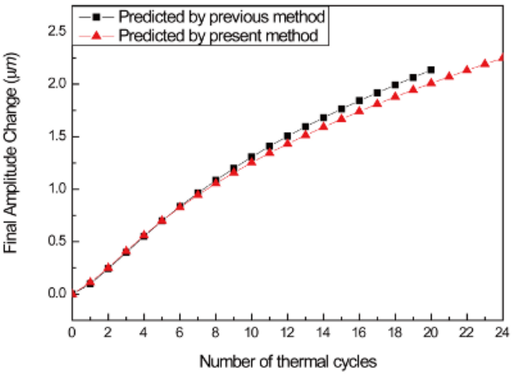

Fig. 16. The comparison of the final amplitude change in surface groove between from the previous method and the present method.

thermal expansion occurring in only one layer of elements. As the thermal cycle continues, TGO thickness therefore increases and those elements simulating TGO thickening should become slender and slender as a result of strain increase in thickness direction. It could be estimated that, as the increased TGO thickness attains a certain value, the previous method will fail to predict the results due to the much geometric nonlinearity exhibited by the expansion element layer. And, the critical value of increased TGO thickness could have been mentioned in [1] wherein the increased TGO thickness should be less than the initial TGO thickness, which is proven by Fig. 16 where the TGO thickness at which the analysis stops is around 1.0 μm. While in the present method, the TGO thickening is simulated simply by changing the material property of substrate into TGO property cycle by cycle, which is free from the large deformation of TGO. For the first few thermal cycles, since the increased TGO thickness is rather thin, the slenderness of the mesh layer is also small enough to be totally accepted by the finite element codes. Consequently, the results for two methods resemble closely illustrating the consistency of two methods in simulating for the small increased TGO thickness. As TGO thickness increases, the meshes in the previous method become more slender so that the predicted value of the amplitude change by the previous method is obviously larger than that by the present one because the mesh for the former expands much more in thickness direction than the latter.

6. Conclusions

A series of finite element analyses have been performed to investigate the displacement instability of surface groove using an improved method which takes account of TGO lateral growth strain and the TGO thickening based on the actual thickness of TGO formed at each thermal cycle. The finite element analyses have used as many as possible in-house measured material parameters with the assumption of material properties to be minimized. Consequently, a quantitatively good agreement with the experiment has been achieved. A special technique is used to simulate TGO thickening. Although the difference between the results by the technique and previous one is not so significant, it shows that the present method can break through the limitation of the TGO thickness, and it can still work for any TGO thickness. Consequently, this work builds a basis for future work, such as analysis of thermo-mechanical cycling, parametric study of various geometry and material factors.

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Jun Ding received his B.S. degree in Mechanical Engineering from Chongqing Institute of Technology, China, in 2000. He then received his M.S. degree from Chongqing University, China, in 2004. Currently a Ph. D candidate at the Graduate School of Mechanical Systems Engineering at Chonnam National University in Gwangju, Korea, he is mainly working on the theoretical and numerical analyses of mechanical behaviors of various materials.

Feng-Xun Li received his B.S. degree from the Department of Mechanical Engineering of Yanbian University, China, in 2005. He then received his M.S. degree from Chonnam National University, Korea, in 2007. He is currently a Ph. D candidate at the Graduate School of Mechanical Systems Engineering at Chonnam National University in Gwangju, Korea and is mainly working on the deformation mechanism of thermally grown oxide.

Ki-Ju Kang received his B.S. degree in Mechanical Engineering from Chonnam National University, Korea, in 1981. He then received his M.S. and Ph.D. degrees from Korea Advanced Institute of Science and Technology in 1983 and 1988, respectively. Dr. Kang is currently a Professor at the School of Mechanical Systems Engineering at Chonnam National University in Gwangju, Korea. His laboratory is designated as a national research laboratory. His research interests include the optimal designs and manufacturing technologies of various types of porous cellular metal and mechanical behaviors of a thermally grown oxide at high temperature.