

Finite Element Simulation of Thermal Barrier Coatings in Rocket Engines

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Abstract: Rocket engines need to withstand extreme gas temperatures. To achieve this, the engine is lined with copper and cooled with liquid hydrogen. Nevertheless, creep processes can lead to damage and failure of the component. To avoid this, rocket engines can be protected with thermal barrier coatings. Standard coating systems as used in gas turbines are problematic because of larger thermal stresses between the copper substrate and the coating due to a large thermal mismatch. In this work, we use finite element simulations to study the stress evolution in a coating material tailored for application in a rocket engine. The influence of the thermal conductivity on the resulting stress state is discussed and general conclusions for the design of thermal barrier coatings in rocket engines are drawn.

Keywords: Coatings, Thermal Stress, Aerospace, Rocket Engine

1. Introduction

The combustion chamber in rocket engines is exposed to high thermal and thermomechanical loads. The process gas can reach temperatures of 3200°C (Greuel, 2002). Since no industrial material can withstand these temperatures, the rocket chamber is lined with copper and cooled on the inside using liquid hydrogen in cooling channels with temperatures of approximately -240°C. The surface temperature of the copper liner can reach temperatures of up to 600°C (Raj, 2007) with large heat fluxes of more 100 MW/m² (Popp, 1996, and Quentmeyer, 1977). The copper liner above the cooling channels has a thickness of 1mm so that the thermal gradient and the large pressure difference between combustion chamber and cooling channel cause a high thermo-mechanical load. This load and thermo-mechanical fatigue cause failing due to the so called dog-house effect (Figure 1) where cooling channels deform visco-plastically, leading to fracture of the copper liner after a few thermal cycles (Riccius, 2004).

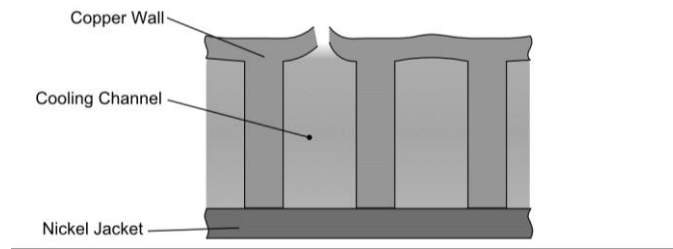


Figure 1. Dog-house effect

In gas turbines, where the process gas is also hotter than the service temperature of the turbine blade material, thermal barrier coatings are used to reduce the thermal load and thus the mechanical stresses. These coatings comprise two layers: a so-called bond coat (usually a NiCrAlY alloy) serves as oxidation protection and improves the adhesion of the top coat material (yttria-stabilized zirconia) that serves as thermal protection (Bürge, 2011).

A similar protection method might also be used in rocket engines, coating the copper liner with a material with lower thermal conductivity and higher service temperature. However, directly transferring the thermal barrier coating systems used in gas turbines to rocket engines is not feasible (Schloesser, 2011) because the very low thermal conductivity of zirconia would lead to extremely high surface temperatures. Furthermore, the coefficient of thermal expansion differs widely between a standard NiCrAlY coating and the copper substrate (see also Figure 5 below), so that high thermal stresses occur at the interface between the copper substrate and the coating.

Therefore, a new coating system needs to be developed that is suitable for the application in rocket engines. Adding copper to a standard NiCrAlY alloy increases the coefficient of thermal expansion and thus reduces the thermal stresses between substrate and coatings. The thermal conductivity of NiCrAlY is already roughly one order of magnitude smaller than that of copper. Furthermore, the service temperature of standard NiCrAlY in gas turbines is approximately 1100°C, much higher than the allowed temperatures in copper alloys. Therefore, a NiCuCrAl coating can possibly serve both as thermal barrier coating and as bond coat.

To evaluate the feasibility of this coating system, it is important to understand the conditions inside the coating and especially the thermal stresses at the interface and inside the coating. Experimentally, this can be done using a laser testing bay described in section 2. A finite element model is used to determine temperatures and stresses inside the coating and to estimate the conditions inside a rocket engine, where component tests are costly to perform.

2. Experimental conditions

Due to the extreme conditions inside a rocket engine and to the high costs of full-scale tests, it is not feasible to perform a large number of experiments using rocket engine experiments. To test thermal barrier coatings under realistic conditions, a laser test bed was constructed, consisting of a 3 kW diode laser with a special optics to produce a broad focal point with 20 mm diameter. To

ensure optical coupling between the specimen and the laser light at a wave length of 808 nm, the specimen can be coated using Fe_3O_4 . In this way, the surface of plate shaped specimens can be heated up to 1500°C in less than 0.8 s. Surface temperatures are measured using a two-color pyrometer. To study cyclic loading of the coatings, the procedure is repeated up to 50 times. Specimens can then be metallographically prepared to study the interface between coating and substrate and to understand failure mechanisms. The experimental setup and results for standard thermal barrier coating systems are described in detail in (Schloesser, 2011).

To understand the failure mechanisms of the coatings, it is necessary to know the conditions at the interface during the cycling experiments. Stresses are generated due to the thermal mismatch of the expansion coefficients of the materials and are exacerbated by the roughness of the interface. Since the interface region is not accessible for measurements during the experiments, finite element simulations are used to calculate temperatures and stresses at the interface.

To transfer the results to the condition inside a rocket engine, a fully coupled fluid-structure model of a rocket engine is used (Kowollik, 2011 and Kowollik, 2013). The calculation shows that a steady state is reached after 0.3 s if a copper substrate with a $100\text{ }\mu\text{m}$ NiCrAlY coating is used. This calculation can then be used to determine the heat transfer between the coating and the hot gas and between the copper substrate and the cooling channel. For this, a simple one-dimensional model is used (Bürge, 2011). The calculated mean film coefficient on the hot-gas side is $\alpha_h=63.5\text{ kWm}^{-2}\text{K}^{-1}$, the cooling-surface film coefficient is estimated as $455.7\text{ kWm}^{-2}\text{K}^{-1}$.

Using these numbers, the temperature of the coating's surface and of the coating-substrate interface can be estimated for different coating thickness as a function of the thermal conductivity of the coating, see Figure 2.

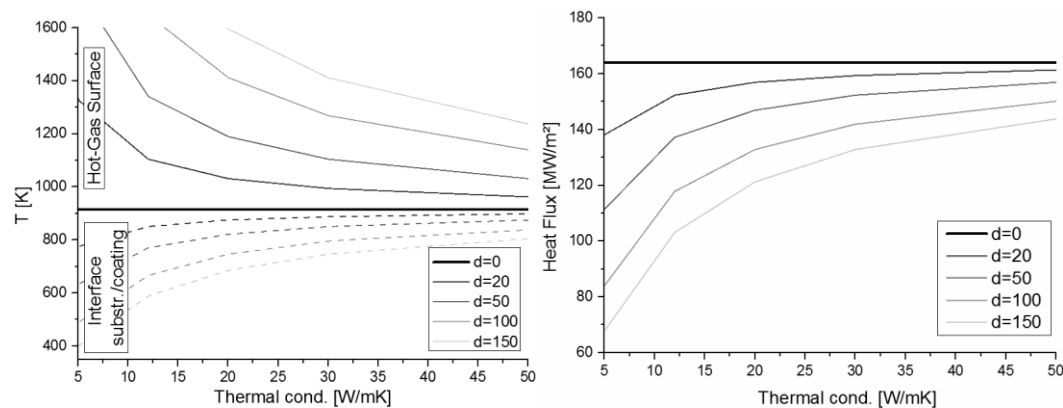


Figure 2 Temperatures and heat fluxes calculated for different values of thermal conductivity and different coating thickness d.

Although this is only an estimate because the film coefficient is assumed not to depend on the coating, the plot shows that a coating with low thermal conductivity will lead to prohibitively high

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surface temperatures, since even ceramic thermal barrier coatings cannot withstand surface temperatures of more than 1200°C (Bürge, 2011). If a coating thickness of 100 μm is assumed, the thermal conductivity should not fall below $\sim 20 \text{ W/mK}$ to keep the surface temperature sufficiently small. This leads to a reduction of the maximum substrate temperature of $\sim 200 \text{ K}$.

3. Finite element model

3.1 Model Description

The two-dimensional geometry of the finite element model was created using the Python scripting interface of Abaqus/CAE. An input deck was written and was directly modified for the variation of boundary conditions and material properties. All calculations were performed using Abaqus/Standard.

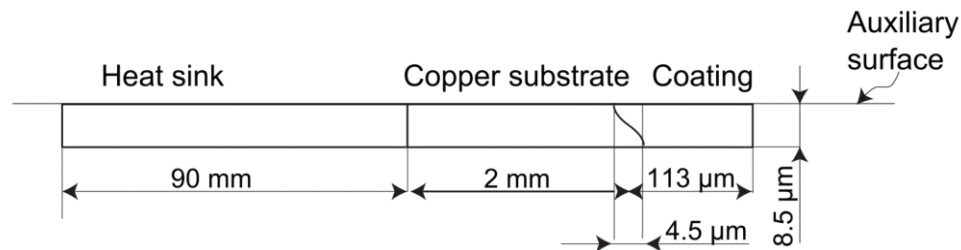


Figure 3. Two-dimensional model geometry

The two-dimensional model geometry is shown in Figure 3. The model consists of a copper substrate with a height of 2 mm (laser testing) or 1 mm (rocket combustion chamber) and a coating with a thickness of 113 μm . The interface between the materials is assumed to be sinusoidal in shape to model the typical interface roughness due to a thermal spraying process (Freborg, 1998). The model is assumed to represent a small strip of material taken out of a large specimen. To ensure correct boundary conditions, the lower edge of the model is restricted in y-direction, whereas the upper edge of the model is tied in normal direction to straight a rigid surface that can only move in the y-direction. These boundary conditions allow for thermal expansion in the y-direction with distorting the shape of the strip of material. In the z-direction, a generalized plane strain condition is assumed.

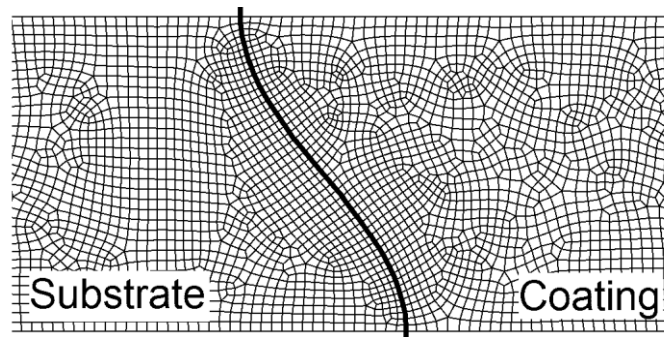


Figure 4. Mesh at the interface substrate/coating

In the laser experiment, the copper specimen is placed on a nickel block that serves as a heat sink. This heat sink was included in the same part. The Young's modulus of the heat sink material was set to a small value (1 MPa) and its coefficient of thermal expansion was set to that of copper so that the thermal stresses in y- and z-direction generated by the heat sink material are negligible.

The specimen was meshed using CPEG4RHT elements. 22000 elements were used in the copper substrate and the coating, using mesh refinement near the interface to resolve the stresses, see Figure 4. The model including the heat sink contained an additional 130000 elements in the heat sink and the extended copper-substrate. Linear elements were chosen to allow for a very fine mesh at the interface with reasonable computational costs. Reduced integration helps to avoid problems due to shear locking since elements at the sinusoidal interface experience some bending. For the purely elastic simulation done here, hybrid elements are not necessary; these elements were chosen because in future simulations creep will be considered and large plastic deformations can be better represented by hybrid elements.

3.2 Material properties

Since the laser testing times are extremely short, no creep of the materials was considered. A purely thermo-elastic simulation was sufficient to estimate the stresses at the interface. Material properties for the copper substrate are taken from (Kupferdatenblatt, 2005, and Dies, 1967, and Fassin, 2015). Material properties of the NiCrAlY coatings are taken from (Pawlowski, 2008, and Altun, 2008, and Taylor, 2004, and Rösler, 2004). Since NiCuCrAl is a new material, the properties have to be estimated. The CTE was measured at the bulk material (Fiedler, 2014), but it is estimated that it will not differ much from the CTE of the NiCuCrAl coating, since the coatings are dense (porosity < 1%). Figure 5 shows the values of CTE for the copper-substrate, the NiCrAlY alloy and the NiCuCrAl alloy. It can be seen that adding 30% copper increases the CTE and will thus reduce thermal stresses at the interface. It is also apparent that the largest thermal stresses will occur at intermediate temperatures of about 900-1000 K.

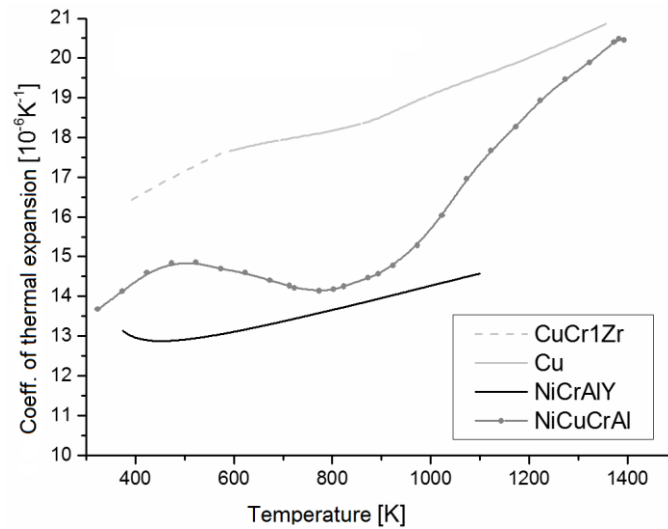


Figure 5. Thermal expansion coefficients related to 273 K

For the heat transfer analysis and the determination of the surface-temperatures, the thermal conductivity is of importance: The thermal conductivity of the Cu-substrate is approximately 320 W/mK. For NiCrAlY it is 12 W/mK at 800 K and 17 W/mK at 1300 K. The thermal conductivity of the NiCuCrAl coating has not been measured so far. Therefore, a parametric study with different thermal conductivities is carried out.

3.3 Thermal boundary conditions

For the simulation of the laser experiment, the left edge of the heat sink was set to a fixed temperature of 293.14 K. The surface of the specimen was heated within 1 second to the final temperature of 1287.84 K, using the temperature profile that was determined pyrometrically in the laser experiments.

To determine the temperature profiles and stresses during exposure for longer times in rocket applications, film coefficients and sink temperatures for heat transfer were provided on the coating-surface and the downside of the copper-substrate based on the calculations in section 2. The hot-gas temperature at the coating surface was set to 3502 K with a film coefficient of $63.5 \text{ kWm}^{-2}\text{K}^{-1}$. At the cooling site of the copper substrate, the sink temperature of the liquid hydrogen was set to 40 K, using a film coefficient of $455.7 \text{ kWm}^{-2}\text{K}^{-1}$.

4. Results

4.1 Laser cycling experiments

During laser cycling, thermal stresses build up at the interface between the copper substrate and the coating. Delamination on the micro-scale usually occurs by crack formation in a direction parallel to the interface, so that the 11-component of the stress is most relevant. Figure 6 shows

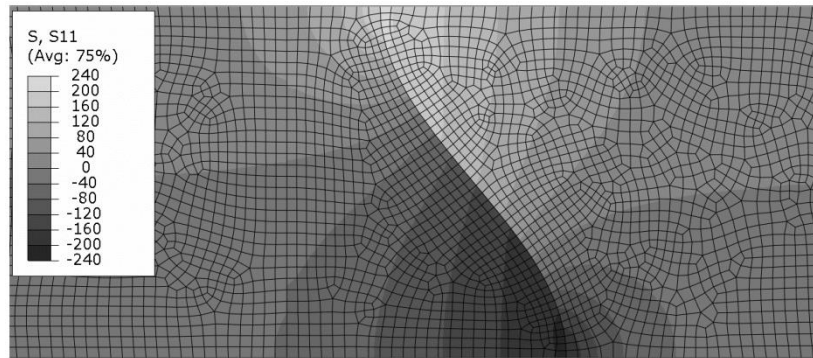


Figure 6. Stress S11 in MPa at the interface substrate (left) and coating (right) for the NiCrAlY coating at 1273 K

this stress component for the case of a standard NiCrAlY coating on copper. Since the CTE of copper is larger than that of the coating, tensile stresses build up in the so-called “valley” region of the interface roughness (upper side in Figure 6). These stresses may cause delamination and failure. Experimentally, it was found that a NiCrAlY coating fails after several thermal cycles due to delamination (Schloesser, 2011).

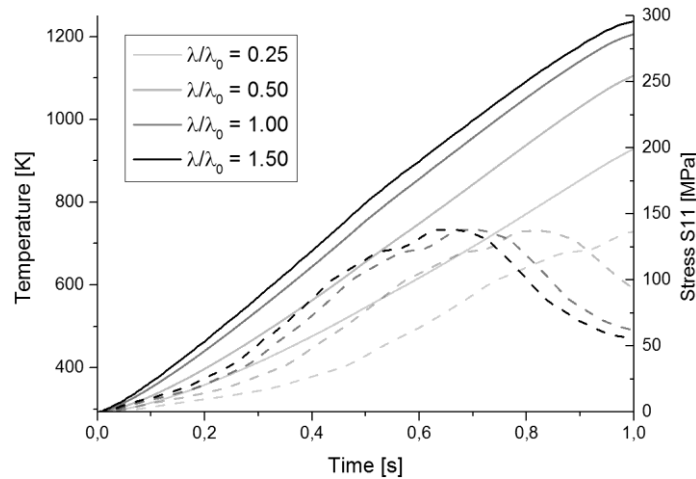


Figure 7. Simulation of the laser experiment with a NiCuCrAl coating: Temperature (solid line) and Stress S11 (segmented line) in the valley of the interface roughness-profile for different values of the thermal conductivity λ ; the reference thermal-conductivity of NiCrAlY is named λ_0 .

The thermal stresses are due to the CTE mismatch between copper and NiCrAlY. If copper is added to the coating material, the CTE significantly increases, leading to a reduction of the thermal stresses. Since the thermal conductivity of NiCuCrAl is not known, simulations with different values of the thermal conductivity were performed, setting the conductivity to 150%, 100%, 50%, and 25% of the value in NiCrAlY.

Figure 7 shows the development of the stress and the temperature at the valley position of the interface region for a NiCuCrAl coating. Although the temperature history depends on the thermal conductivity, the maximum stresses are very close and occur at an interface temperature of about 950K. The reason for this is that the difference of the CTE between copper and NiCuCrAl becomes smaller at higher temperatures, see Figure 5.

Figure 8 shows the stress history at the valley region for a NiCrAlY and a NiCuCrAl coating, both with a thermal conductivity of NiCrAlY. It is apparent that the maximum stresses are strongly reduced when copper is added to the coating material. If creep is considered, the reduced stresses will also lead to a smaller amount of visco-plastic deformation so that residual stresses after

cooling to room temperature would be reduced as well. From this point of view, adding copper to the coating material should serve to improve the lifetime of the coating.

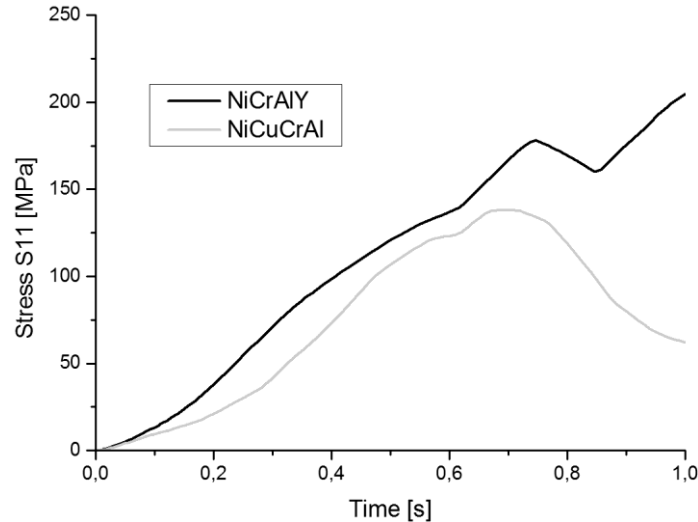


Figure 8. Simulation of the laser experiment: Stress S11 for a NiCrAlY and a NiCuCrAl coating

4.2 Simulation of a rocket engine

The laser testing experiments are temperature-controlled because the laser power is directly controlled using the measured surface temperature. Inside a rocket engine, changing the coating material's thermal conductivity will also affect the temperature profile and the maximum temperatures, see also Figure 2. The second model (see section 3.1) has been used to study the effect of the thermal conductivity when the sink and gas temperature and the film coefficient are fixed (see section 3.3).

Figure 9, left shows the surface temperature of the coating and the interface temperature for a NiCuCrAl material with different heat conductivities. If the thermal conductivity is too small, the surface temperature of the coating is far beyond the service temperature of nickel-based materials. Even a large thermal conductivity still leads to rather high surface temperatures of 1400 K. However, this does not imply that NiCuCrAl cannot be used as a coating system because the thickness of the coating was kept fixed in the simulation. A coating thickness of 100 μm , as assumed here, reduced the temperature of the interface region to values below 700 K, which is below the values reached in the laser cycling experiments. Therefore, a thinner coating might be used.

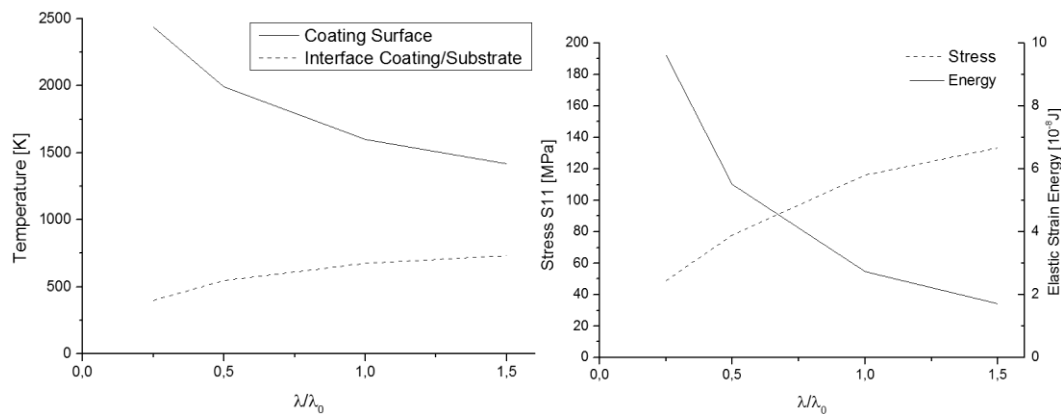


Figure 9. Temperature, maximum Stress S11 at the substrate/coating interface and elastic strain energy in the coating for different values of the thermal conductivity λ , the reference thermal-conductivity of NiCrAlY is named λ_0 .

Figure 9, right shows the maximum stress S11 at the interface region. As expected, the maximum stress occurs for the highest thermal conductivity of the coating, but absolute values are still below 150 MPa and will probably not be sufficient to cause significant delamination.

However, failure of a coating system may also be affected by buckling of the coating due to large compressive stresses in the in-plane directions. Buckling is driven by the stored elastic energy. Since the stresses in 22- and 33-direction are considerably larger than the 11 stresses except directly at the interface, the total stored energy inside the coating can be used as a rough indicator of the tendency of the coating to buckle. (Note that this is only an estimate because the stresses in 22- and 33-direction are tensile near the interface and will thus not contribute to buckling, but may instead cause segmentation cracks. Since these cracks might also reduce the lifetime and increase the probability of delamination, a large value of the total stored elastic energy can be considered unfavorable.)

Figure 9, right shows the total stored elastic energy inside the coating. As expected, the energy becomes smaller with increasing heat conductivity because the copper temperature increases so that the thermal stresses inside the coating are reduced.

5. Discussion and Conclusions

The results presented here show that adding copper to a NiCrAlY coating system is very likely to improve the lifetime of the coating on a copper substrate. Thermal stresses at the interface are strongly reduced compared to the case of a standard NiCrAlY alloy. Furthermore, it can be expected that the adhesion will be improved if copper is present in the coating.

Simulations using the rocket engine model show that the – so far unmeasured – thermal conductivity of the coating material must not be too small to avoid extreme surface temperatures

and to increase the copper temperature because otherwise large thermal stresses will develop inside the coating that may lead to buckling or segmentation cracks.

Depending on the actual thermal conductivity of NiCuCrAl coatings, a coating consisting of only this material may not be feasible because the thermal gradients in the coating would be large and surface temperatures might be extreme. However, NiCuCrAl would still be highly useful as a bond coat material on which a second top coat is applied. The simulations shown here already allow to draw some conclusions on the desired properties of the top coat material: (i) its service temperature should exceed that of NiCuCrAl; (ii) its thermal conductivity should be sufficiently large (at least as large as that of NiCrAlY) to avoid extreme surface temperatures; (iii) the coefficient of thermal expansion should lie below that of NiCuCrAl so that thermal mismatch stresses in the 22- and 33-direction that might cause buckling are reduced (ideally the CTE value should be chosen so that the mean thermal strain at the high coating temperature is comparable to the mean thermal strain inside the copper material). Further finite element simulations including a top coat will be performed in the future to facilitate the material selection of the top coat.

6. References

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