INTRODUCTION

Thermal barrier coatings (TBCs) for gas turbine hot section components were developed to establish a thermal gradient between the hot gas and the metallic substrates. This allows either to increase the hot gas inlet temperature to improve the turbine efficiency or to extend component lifetimes by reducing thermal loads. Both of these aspects motivated researchers within this field to find novel TBC materials to overcome the shortcomings of the state-of-the-art yttria partially stabilized zirconia (YSZ). YSZ decomposes at elevated temperatures (>1200°C) into high-yttria- and low-yttria-content zirconia phases.1,2 The low-yttria zirconia transforms upon cooling into the monoclinic phase with an associated large volume expansion of ~4%, which can lead to the failure of the TBC systems.3 Among the large number of alternative candidates for new generation TBC materials, complex rare-earth perovskites with the general formula A(B'B″)O3 have gained particular interest.4 Ba(Mg1/3Ta2/3)O3 has an extremely high melting point of approx. 3100°C 5 and exhibits an advantageously high coefficient of thermal expansion (CTE) value (10.9 × 10−6/K at 30°C-1000°C) for TBC applications.6 Another interesting characteristic of these complex perovskites is the ordering effect of the B-site cations, which enables tailoring of materials properties.7 Recently, plasma-sprayed La2(Al1/2MgTa1/2)O6 (LAMT) showed significantly improved thermal cycling lifetime results, when applied in a double layer TBC system on top of a YSZ basis to compensate the rather low fracture toughness of LAMT.6,8 In addition to materials aspects, the lifetime of...
TBCs can also be improved by various microstructural features like the presence of vertical cracks or highly porous columnar microstructures obtained by the suspension plasma spraying (SPS) technique. With such kind of microstructures, TBCs can better tolerate high thermal stresses during operation. Interestingly, after a long-term thermal cycling test, in which a LAMT/YSZ TBC system was exposed to repeated heating \( (T_{surface} \approx 1390^\circ C \text{ for } 5 \text{ minutes}) \) and cooling \( (T_{surface} < 100^\circ C \text{ for } 2 \text{ minutes}) \) cycles, the LAMT layer close to the surface was completely transformed to \( \text{La}_3\text{TaO}_7 \) phase, which, however, did not deteriorate the cycling performance. This secondary phase was probably formed due to the evaporation of volatile species such as MgO and Al\(_2\)O\(_3\), showing higher vapor pressures than those of the other components in LAMT. The initial formation of this secondary phase obviously takes place already during the spraying process. The XRD pattern of the as-sprayed coating surface revealed, beside the initial single-phase LAMT powder, an amorphous hump with a few significant crystalline peaks which correspond well to the strongest peaks of the \( \text{La}_3\text{TaO}_7 \) phase. The failure of the SPS LAMT coating was initiated at the interface of TBC and metallic bond coat which protects the substrates from oxidation and provides improved bonding between the substrate and the TBC layer. Due to the formation of thermally grown oxides (TGO) at this interface, additional stress is induced in the system and the crack growth can easily propagate along these oxides. Since this detaching of the TBC system only took place at the interface and not inside the LAMT coating itself, the thermal stability of LAMT, somehow, obviously also contributes to the long-term cycling performance in addition to the microstructural effects.

From materials point of view, LAMT is a promising candidate for TBC application. Yet, little is known about its detailed crystal structure or phase transitions so far. Up to now, the synthesized single-phase LAMT powder was described by an orthorhombic phase at room temperature which is isostructural to \( \text{LaFeO}_3 \). The Pawley refinement on the XRD data showed no peculiarity in the orthorhombic cell symmetry. No crystal structural information is used during the Pawley refinement to predict the peak intensities, and only unit cell, peak profile, and variable intensity parameters are used in a traditional iterative least squares refinement. This procedure allows a fast determination of the unit cell parameters and gives an optimized peak profile description of the observed powder pattern.

However, when trying a Rietveld refinement using the \( \text{LaFeO}_3 \) as a starting crystal structure model, in which the \( B \)-site atom Fe on the \( 4b \)-Wyckoff position was replaced by Al, Mg, Ta, with its site occupancy factors of 1/4, 1/2 and 1/4, respectively, a strong mismatch between the observed and calculated Bragg peak intensities was found. Since the Bragg peak intensities are now constrained by a chosen crystal structure in the calculation, such a strong intensity mismatch can suggest that the chosen crystal structure is not correct. Another reason for intensity deviation can be assigned to a texture effect. This was excluded owing to the powder morphology, as well as, by trying out different sample preparation methods. Various sample holders were tested to pack or distribute the powder in a texture-free way. However, the intensity ratios did not vary much, and showed almost the same ratios. Moreover, the refinement ended up with unphysically distorted \( B \)-site octahedra in this orthorhombic cell setting. Assuming that the orthorhombic crystal structure is incorrect, another crystal structure model reported earlier for \( \text{La}_2\text{Mg}(\text{Mg}_{1/2}\text{Ta}_{2/3})\text{O}_6 \) was chosen for the room-temperature phase of LAMT. Whereas the orthorhombic unit cell describes a completely disordered arrangement of the \( B \)-site cations, the monoclinic unit cell (corresponding to a subgroup of the orthorhombic cell) gives a rock-salt type ordering of the \( B \)-site cations. It is well-known, that, in these double perovskite \( A_b\text{B}_b\text{O}_6 \) compounds, the \( B \)-cations tend to order over long range if their difference in oxidation state or size is large enough. \( B \)-cations of LAMT exactly fall into these categories with their oxidation state as well as difference in ionic radii of Al\(^{3+} \) (\( r = 0.53 \) Å, coordination number (CN) = 6), Mg\(^{2+} \) (\( r = 0.72 \) Å, CN = 6), and Ta\(^{5+} \) (\( r = 0.64 \) Å, CN = 6). A similar \( B \)-cation ordering was also reported for \( \text{La}_x\text{CrMg}_{2/3}\text{Nb}_{1/3}\text{O}_6 \) using selected area electron diffraction (SAED) patterns, where forbidden reflections for the orthorhombic symmetry (space group, \( Pnma \)) were clearly observed which are allowed in the monoclinic symmetry (space group, \( P2_1/n \)).

Regarding thermal stability of single-phase LAMT, dilatometry measurements showed no evidence for significant structural phase transition up to 1200°C. Thus, the present work tries to develop an improved understanding of the crystal structure and the phase transitions for LAMT using in situ HT-XRD up to 1430°C, complemented by DSC/TG measurements up to 1500°C.

### 2 | EXPERIMENTAL PROCEDURE

#### 2.1 | Powder synthesis

LAMT powder was synthesized from stoichiometric amounts of \( \text{La}_2\text{O}_3, \text{Al}_2\text{O}_3, \text{MgO}, \text{and} \text{Ta}_2\text{O}_3 \) powders. The mixture was suspended in ethanol and mechanically ground by ball milling at 150 min\(^{-1} \) for 12 hours. The precursors were then dried and calcinated at 1250°C for 3 hours, and after an additional ball milling process at 150 min\(^{-1} \) for 48 hours, the powder was heat-treated at 1600°C for 4 hours. The synthesized LAMT powder was single-phase according to the powder XRD measurement.

#### 2.2 | HT-XRD

HT-XRD was conducted at an X-ray powder diffractometer, Empyrean (Malvern Panalytical GmbH) using a HTK1200N environmental heating chamber (Anton Paar GmbH) up to 1000°C and a HTK16N direct heating chamber (Anton Paar
Temperature up to 1430°C with intervals of 100°C. Temperature of both heating chambers was calibrated using a pure CeO$_2$ powder (Sigma-Aldrich, 99.995%). The CTE derived from the lattice parameters was then validated as a function of temperature corresponding to the well-established literature value$^{15}$ (considered accuracy within ±5%). The heating and cooling rate of the sample was 5°C/min. At each temperature, the XRD data were collected in Bragg-Brentano geometry using CuK$_{\alpha 1,2}$ radiation (45 kV/40 mA), in the 2θ range of 17°-100° with Δ2θ = 0.026° and counting time of 100 seconds using a 255 channel position-sensitive PIXcel detector. Rietveld analysis of the data was performed using the TOPAS program V4.2 (Bruker AXS)$^{16}$.

2.3 | DSC/TG

The DSC/TG measurements were carried out with a Netzsch STA 449 F3 apparatus with a rhodium furnace in the temperature range between 25°C and 1500°C with a heating and cooling rate of 30°C/min. LAMT powder sample of ~81 mg was prepared in a platinum crucible (Pt 97%: Ir 3%) covered by a lid. Repeated measurements were performed under the same experimental conditions with each powder being freshly prepared in order to check the reproducibility.

3 | RESULTS AND DISCUSSION

3.1 | Crystal structure analysis through Rietveld refinement

The Rietveld refinements based on powder XRD data on single-phase LAMT revealed a monoclinic, rhombohedral, and cubic phase symmetry at 25°C, 1155°C, and 1430°C, respectively. Observed, calculated, and difference patterns (Yobs, Ycalc and Yobs-Ycalc) of the Rietveld refinements are shown in Figure 1 with corresponding Bragg peak positions for the given crystal structure. Insets are also added to better represent the significantly different XRD patterns of the rhombohedral and cubic LAMT phases (Figure 1B,C).

As already mentioned in the introduction, the B-site cation ordering effect lowers the symmetry of the unit cell, and the room-temperature phase of LAMT crystallizes in a monoclinic unit cell. Compared to the orthorhombic unit cell with the space group Pnma, the weighted R-value of the monoclinic one improved significantly from $R_{wp}$ (Pnma) = 7.63 to $R_{wp}$ (P2$_1$/n) = 4.55, with 23 and 29 refined parameters, respectively. Moreover, the atomic displacement factors converged to a positive value in the monoclinic cell whereas they ended up with an implausible negative value in the orthorhombic cell. The strong distortion of BO$_6$ octahedra, which gave no reasonable bond lengths and angles in the orthorhombic cell, also diminished considerably in the monoclinic cell. The results of Rietveld analysis at each temperature are summarized in Table 1.

![Rietveld refinements of powder XRD data (CuK$_{\alpha 1,2}$ radiation) on single-phase LAMT at (A) 25°C, (B) 1155°C, and (C) 1430°C. Insets show the correspondingly indexed Bragg peaks for the rhombohedral (subscript r) and the cubic (subscript c) LAMT phases.](Color figure can be viewed at wileyonlinelibrary.com)

Using TOPAS V4.2 (Bruker AXS)$^{16}$ fundamental parameters with microstructure effect (size and strain) were applied to describe the peak profile. Some constraints were
needed during Rietveld refinement. The atomic displacement parameter was constrained to the same value for all the B-site atoms and also for all the oxygen atoms, respectively. Based on the ICP-OES (inductively coupled plasma optical emission spectrometry) result, the chemical composition of LAMT powder was confirmed to be within the error range. Therefore, the site occupancy factor of B-cations was fixed to be Al:Mg:Ta = 0.5:1:0.5 in the refinement.

Unit cells of LAMT phases at different temperatures are visualized in Figure 2 with views along given [uvw]-directions related to the corresponding basis vectors in each unit cell setting. As illustrated in Figure 2, the B-site cations are ordering in a rock-salt type arrangement in each unit cell. The large differences in the ionic radii (Mg²⁺ > Ta⁵⁺ > Al³⁺) as well as in the oxidation state apparently favor an ordering of the B-site cations as reported earlier. For the occupancy of the B-site,

**TABLE 1** Results of Rietveld analysis on single-phase LAMT at different temperatures

| Temperature (°C) | 25 | 1155 | 1430 |
|------------------|----|------|------|
| Crystal system, space group | Monoclinic, \( P2_1/n \) | Rhombohedral, \( R \bar{3} \) | Cubic, \( Fm\bar{3}m \) |
| \( a, b, c (\text{Å}), \beta (^\circ) \) | 5.569 (3), 5.571 (3), 7.870 (3), 90.07 (3) | 5.648 (1), −13.793 (4), − | 8.030 (1), −, −, − |
| \( V (\text{Å}^3) \) | 244.2 (2) | 381.1 (2) | 517.9 (2) |
| \( Z \) | 2 | 3 | 4 |
| \( D (\text{g/cm}^3) \) | 6.83 | 6.56 | 6.44 |

**Atomic parameters**

| | \( x \) | \( y \) | \( z \) | Occ. | \( B_{\text{iso}} \) |
|---|---|---|---|---|---|
| La | 0.5032 (9) | 0 | 0.2508 (9) | 1 | 1.52 (2) |
| Al/Ta | 0.5 | 0 | 2498 (2) | 0.5 |
| Mg | 0 | 0.5 | 0 | 0 |
| Al/Ta | 0 | 0 | 0.5 | 0.5 |
| Mg | 0 | 0 | 0 | 0 |
| O1 | 0 | 0.216 (6) | 0.341 (1) | 0.2491 (4) |
| O2 | 0 | 0.221 (6) | 0.119 (2) | 0 |
| O3 | 0 | −0.020 (4) | 0.4182 (7) | 0 |

\( R_w = \sqrt{\sum w (Y_o - Y_c)^2 / \sum w Y_o^2} \), \( \chi^2 = \sqrt{\sum w (Y_o - Y_c)^2 / M - P} \) where \( w = 1/\sigma(Y_o)^2 \), \( Y_o \) observed data, \( Y_c \) calculated data, \( M \) number of data points, \( P \) number of parameters.
we assumed the fully occupied Mg$^{2+}$ only on one of the B-sites and each a half occupation of Ta$^{5+}$ and Al$^{3+}$ on the other B-site. The statistical distribution of the Mg$^{2+}$ ions on both of the B-sites (each a half occupation with Mg$^{2+}$ and the other half with Ta$^{5+}$ and Al$^{3+}$, respectively) gave for all the phases a slightly poorer Rwp value. A noticeable discrepancy was also found in the monoclinic phase between these two B-site cation configurations. The B-site octahedral distortion was larger in the statistically distributed Mg configuration, and less distorted octahedra were formed if one of the B-sites was fully occupied with the Mg$^{2+}$ ions. Other attempted refinement strategies like refining the site occupancies of B-site cations with some restraints implemented, gave the best fit with ordered configuration of the B-site cations. Therefore, the fully occupied Mg$^{2+}$ ions on one of the B-sites were consequently taken as the structure model, presuming that the ordering of the B-site remains throughout the high-temperature phase transitions.

Considering the electrostatic benefits, the separation of the more highly charged Ta$^{5+}$ cation from its nearest lower charged neighbors (Mg$^{2+}$/Al$^{3+}$ cations) is well established through the rock-salt type arrangements. 12,13 Moreover, the ionic radii difference apparently favors the geometrical separation of the large Mg$^{2+}$ ions ($r = 0.72 \text{ Å}$) from the other smaller Al$^{3+}$ ($r = 0.53 \text{ Å}$) and Ta$^{5+}$ ions ($r = 0.64 \text{ Å}$). The corner-sharing $BO_6$-octahedra of LAMT exhibit a strong tilting in the monoclinic and rhombohedral crystal system (Figure 2A,B). Due to the corner-sharing network of the $BO_6$-octahedra, the tilt of one octahedron is directly coupled to the tilting of the adjacent octahedra. The notation developed by Glazer is most commonly used to describe octahedral tilting in perovskites.17 According to the Glazer notation, the monoclinic, rhombohedral, and cubic structures of LAMT are given the symbols, $a^-a^-c^+$, $a^-a^-a^-$, and $a^0a^0a^0$, respectively. The cubic LAMT has no tilt around the $x$, $y$, and $z$ axes, which corresponds to the symbol $a^0a^0a^0$, whereas three-tilt systems exist in the monoclinic and rhombohedral crystal structures of LAMT (Figures 3 and 4). The $a^-a^-c^+$ in the monoclinic system indicates that the rotation angle about the $z$ axis is different from the rotation angle about the $x$ and $y$ axes, and the superscripts “+” and “−” denote the same and the opposite rotation directions in adjacent layers, respectively. Hence, the octahedral tilting in the monoclinic LAMT has the same magnitude around the $x$ and $y$ axes with the opposite relative orientations of adjacent layers and a different magnitude around the $z$ axis with the same relative orientation as depicted in Figure 3 (monoclinic structure). The symbol $a^-a^-a^-$ for the rhombohedral LAMT indicates all the same rotation magnitude in the three Cartesian axes.

![Figure 2](https://wileyonlinelibrary.com)
with the opposite rotating directions. In Figure 4 (rhombohedral structure), the tilt system along one triad axis (view along [001] direction) and one tetrad axis (view along [241] direction that corresponds to a fourfold axis in the cubic unit cell) are visualized.

Selected interatomic distances, bond angles, octahedral tilt angles, $\theta$, $\phi$, as well as bond length distortion (BLD), and octahedral angle variance (OAV)\(^{18}\) of LAMT at different temperatures are given in Table 2. The Al,Ta–O and Mg–O distances as well as the bond angles in the monoclinic LAMT are in good agreement with the reported literature values.\(^{11}\) As the temperature increases, the tilting magnitude decreases and the difference in Al,Ta–O and Mg–O bond lengths diminishes, so that the cubic phase at 1430°C reveals an ideal perovskite structure with almost equal Al,Ta–O and Mg–O distances. By calculating the tolerance factor ($t$)\(^{19}\) of complex perovskites with

$$t = \frac{\langle rA \rangle + rO}{\sqrt{2} (\langle rB \rangle + rO)},$$

where $\langle r \rangle$ is the weighted ion radius\(^{14}\) at the given site, we get $t = 0.951$. Since this value is smaller than 1, we expect an octahedral tilting in this LAMT system. Using the bond lengths of $A$–O and $B$–O calculated from the Rietveld analysis, we get $t = 0.98(3), 0.99(1)$ and $1.000(3)$ for the monoclinic, rhombohedral, and cubic LAMT phases, respectively.

### 3.2 High-temperature phase transitions

Unlike reported earlier through dilatometry measurements,\(^6\) completely reversible structural phase transitions were observed at ~855°C and at ~1390°C upon heating. The XRD patterns of the LAMT powder sample at room temperature after the HT-XRD measurements confirmed the single-phase monoclinic LAMT. The lattice parameters and the unit cell volume changes as a function of temperature between 25°C and 1430°C are represented in Figure 5. The rhombohedral lattice parameters (hexagonal setting) were converted to the monoclinic ones for a better comparison ($a_m = \frac{1}{3} a_h + \frac{1}{3} b_h + \frac{1}{3} c_h$, $b_m = a_h + b_h, c_m = \frac{2}{3} a_h - \frac{2}{3} b_h + \frac{1}{3} c_h$). The unit cell volume changes gradually as a function of temperature without any abrupt jump.

### 3.3 DSC/TG

When LAMT powder was heated with a rate of 30°C/min, an endothermic signal at 865°C was observed (Figure 6). This signal refers to the monoclinic to rhombohedral phase transition. An exothermic signal at 844°C was detected on cooling, and with a presence of a hysteresis, this phase transition has a first-order character. Within our DSC/TG experiments, we could not observe any significant signal of the rhombohedral to cubic phase transition above 1300°C. There was also a limitation in the DSC instrument that a smaller DSC range could not be set.

![Figures 3 and 4](http://wileyonlinelibrary.com)
for more sensitivity in detection. We assume that this rhombohedral to cubic phase transition has a continuous character without any abrupt volume change as reported for a Ba$_2$Bi$_2$O$_6$ compound.$^{20,21}$ Two possible paths of symmetry reduction by group-subgroup relations are depicted in Figure 7.

After 3 hours of annealing LAMT powder at 1600°C in air, no decomposition was found. However, after a long-term heating of 50 hours at 1500°C in air, a secondary phase, LaAlO$_3$ was detected by XRD.

### 3.4 Discussion of the potential application of LAMT in thermal barrier coating systems

Several CTE values of conventional TBC materials from literature and our own experimental values (LAMT and La$_3$TaO$_7$) by HT-XRD are plotted as a function of temperature in Figure 8. The constant CTE change of LAMT without any abrupt jump at phase transitions refers to a continuous reduction of octahedral tilting in the system.

To reduce the effect of thermal mismatch, as well as to compensate a rather weak fracture toughness (as described in Section 1), LAMT was applied as a top layer on a YSZ basis in a double layer TBC system.$^8$ Furthermore, it was manufactured by SPS to obtain a columnar microstructure.$^8$ Such columnar structure is strain-tolerant and shows high porosities, which is favorable to achieve low thermal conductivities.

It is known that the formation of secondary phases during thermal loading can lead to a failure of the system due to a thermal expansion mismatch.$^{24}$ But here, no detaching or failure within the LAMT-TBC system was observed.
Figure 5: Lattice parameters and unit cell volume changes of LAMT as a function of temperature between 25°C and 1430°C on heating. The continuous solid lines are a guide to the eyes. The phase transition temperatures on heating are marked with vertical-dashed lines. [Color figure can be viewed at wileyonlinelibrary.com]
although complete transformation occurred on the surface (La$_3$TaO$_7$) and different phases were present throughout the whole ceramic layer. The very similar CTE values between La$_3$TaO$_7$ and LAMT (Figure 8) in the thermal loading test ranges can explain the thermal stability of this system.

Materials with high thermal stability up to operating temperature without any phase transition or secondary phase formation are desirable. However, as our studies show, the stability of a TBC system should be investigated in more detail taking the role of each new phase found in the system during thermal loading into account. If the contribution of individual phases is profitable to the whole system, for example, by relaxing stress, strengthening bonding or compensating different thermal expansion mismatch, the applied material can be a promising candidate for a TBC system. In this context, fine tunable complex perovskites certainly have significant potential.

4 | CONCLUSIONS

Rietveld analysis on a single-phase LAMT powder revealed the B-site–ordered monoclinic crystal structure with the space group $P2_1/n$ at room temperature. This ordering effect is driven by the large difference in oxidation states as well as in ionic radii of the B-site cations. Upon heating, LAMT undergoes a first-order phase transition at ~855°C, and crystallizes in a rhombohedral crystal structure with the space group $R_3$. This phase transition is reversible, and shows a hysteresis of ~21°C when LAMT was heated and cooled down with a ramp of ±30°C/min.

As expected from the Goldschmidt tolerance factor of LAMT smaller than 1, octahedral tilting occurs in the lower symmetry crystal structures. The magnitude of the octahedral tilting is larger in the monoclinic system, and by approaching a higher symmetry on heating, the degree of tilting decreases, and the B-site octahedra take a more regular form.

The aristotype cubic perovskite structure ($Fm\overline{3}m$) forms at ~1390°C, with a doubling of the unit cell ($a = 8.030(1)$ Å) due to the B-site ordering effect. This phase transition has a second order character and is reversible. There is a group-subgroup relationship between the rhombohedral and the cubic space group symmetries.
High lifetime of LAMT in TBC applications involves the beneficial columnar microstructure formed by the suspension plasma spraying technique, as well as the thermal stability of the material itself with regard to a nondestructive volume change at the structural phase transitions. The structural phase transitions of LAMT are related to a degree of octahedral tilting which decreases with increasing temperature. The continuous reduction in the octahedral tilt angle with increasing temperature is responsible for a smooth CTE development, and hence beneficial for performance under thermal load.

Fine tunable complex perovskites give researchers in this field further opportunity to find promising candidates for TBC systems.

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