

Accepted Manuscript

Title: Mechanism of crack nucleation and growth in YSZ thermal barrier coatings corroded by CMAS at high temperatures: First-principles calculation

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PII: S0010-938X(18)30648-6
DOI: <https://doi.org/10.1016/j.corsci.2018.07.033>
Reference: CS 7632

To appear in:

Received date: 9-4-2018
Revised date: 7-7-2018
Accepted date: 25-7-2018

Please cite this article as: Chen Z, Zheng H, Li G, Li H, Peng P, Mechanism of crack nucleation and growth in YSZ thermal barrier coatings corroded by CMAS at high temperatures: First-principles calculation, *Corrosion Science* (2018), <https://doi.org/10.1016/j.corsci.2018.07.033>

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Mechanism of crack nucleation and growth in YSZ thermal barrier coatings corroded by CMAS at high temperatures: First-principles calculation

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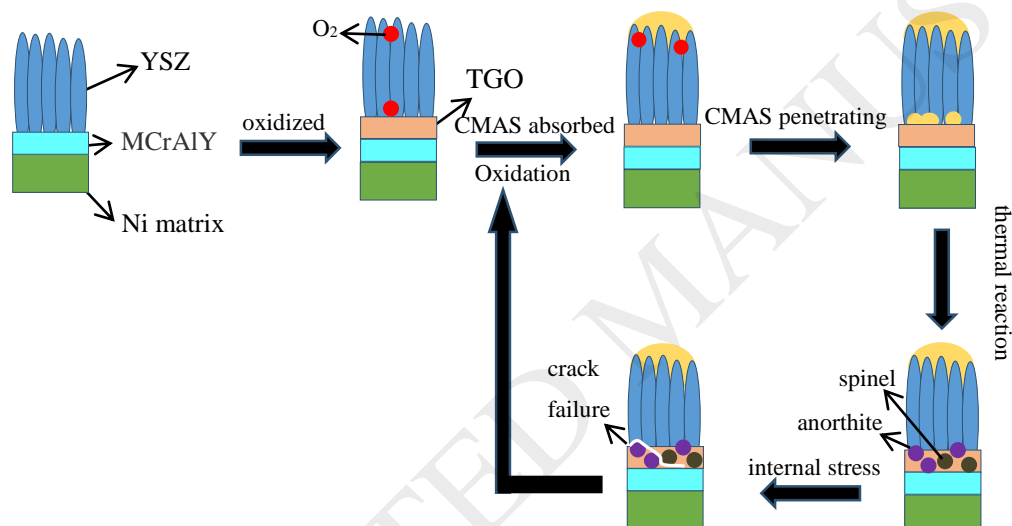
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Graphical abstract



Highlights

- The mechanism of crack nucleation and growth in YSZ TBCs corroded by CMAS is investigated by DFT calculations.
- TGO is advantageous for the protection and bonding of the TBC to the matrix alloy due to its outstanding structural stability and excellent interfacial strength.
- The YSZ/CaAl₂Si₂O₈ interface, possessing the weakest atomic bonds, Zr-O and Ca-O, is the crack nucleation site.
- The difference in thermal expansion coefficients and the low boundary strength between CaAl₂Si₂O₈ and

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