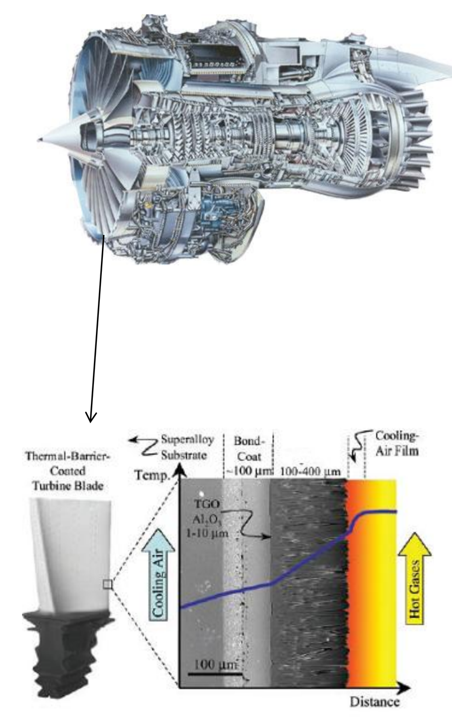
Phase-Field Modeling of the Sintering Process in Thermal Barrier Coating (TBC) Systems

Karim Ahmed, Jie Deng, and Anter El-Azab

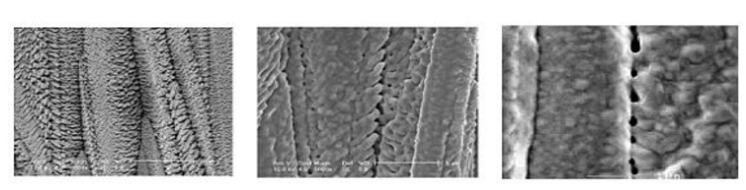
Motivation

Improving efficiency of gas engines and extending their operation time requires increasing inlet temperature.

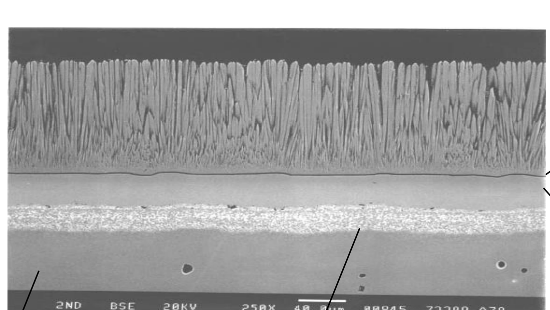


Thermal Barrier Coatings (TBC) are used to extend the lives of substrate alloys by protecting them from high temperature and rapid temperature transients.

Sintering reduces the porosity of the TBC which increases its thermal conductivity and decreases its strain tolerance. So studying the sintering process will pave the way to produce robust and efficient TBC systems



Microstructure of the TBC system



Top coat: provides thermal barrier.

Thermal grown oxidation (TGO): forms as a result of bond coat oxidation, and provides adhesion and oxidation resistance.

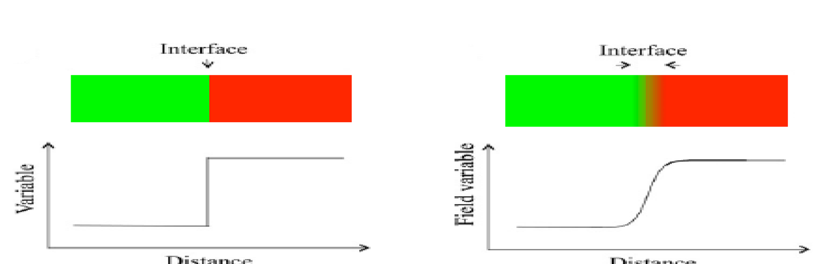
Bond coat: provides bond between top coat and substrate, must be able to form a protective, stable and slow-growing TGO

Substrate: optimizes mechanical properties

Interdiffusion layer

The common substrates are nickel based alloys whereas as the common topcoat is yttria-stabilized zirconia(YSZ).So there is a thermal expansion mismatch that we should take it into account in the model

Phase-Field modeling method



The phase-field method has become an important and extremely versatile technique for simulating microstructure evolution at the mesoscale. Thanks to the diffuse-interface approach, it allows us to study the evolution of arbitrary complex grain morphologies without any presumption on their shape or mutual distribution. It is also straightforward to account for different thermodynamic driving forces for microstructure evolution, such as bulk and interfacial energy, elastic energy and electric or magnetic energy, and the effect of different transport processes, such as mass diffusion, heat conduction and convection

Phase-Field Modeling of Sintering in TBC System

In this model, the microstructure is described by a set of continuous phase field variables (also called order parameters) of two types, conserved and non-conserved. The (normalized) mass density $\rho(r,t)$ is a conserved order parameter giving the distribution of solid materials over the entire material domain. This order parameter is taken to be 1 in the solid and 0 in the pore regions. Non-conserved order parameters η $(r,t;\alpha = 1,2,\ldots, p)$ are used to distinguish different solid regions (e.g., grains with different crystallographic orientations), such that η (α) equals to 1 in α -th grain and 0 otherwise.

The free energy functional of the TBC system can be written as

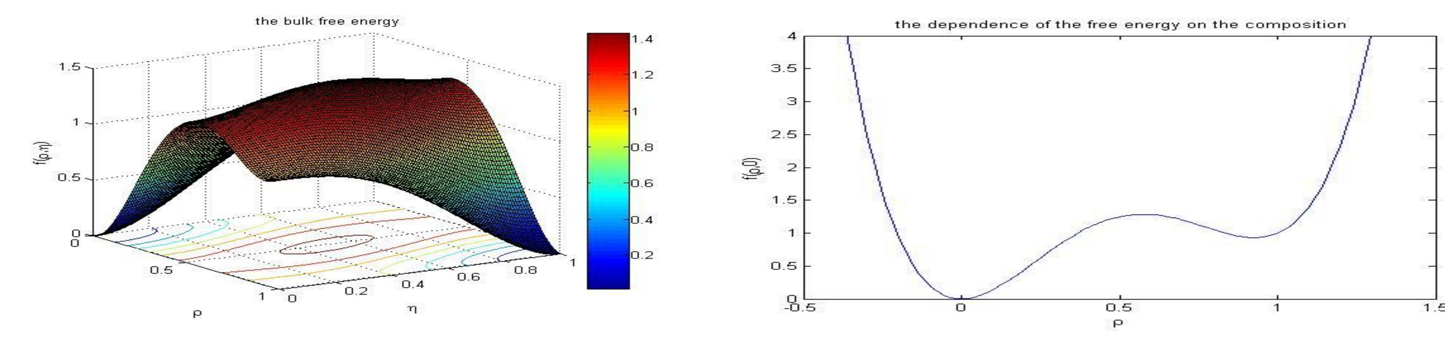
$$F = \int_V \left[f(\rho, \eta_1, \eta_2, \cdots) + e(\rho) + \frac{1}{2}\beta_\rho |\nabla\rho|^2 + \sum_\alpha \frac{1}{2}\beta_\eta |\nabla\eta_\alpha|^2 \right] d^3 r$$

the bulk free energy — the elastic energy — the interface energy

The bulk free energy can be approximated in terms of the order parameters by

$$f = A\rho^2(1-\rho)^2 + B\left[\rho^2 + 6(1-\rho)\sum_\alpha \eta_\alpha^2 - 4(2-\rho)\sum_\alpha \eta_\alpha^3 + 3\left(\sum_\alpha \eta_\alpha^2\right)^2\right]$$

Where A and B are constants. This form of energy density is so constructed that it has multiple minima in different solid and porosity sub-domains. We can easily visualize it if we assume that we have only one grain (i.e. the solid phase is isotropic), then we will have only two minima one is corresponding to the isotropic solid phase and the other is corresponding to the pore phase.



The elastic energy is given by

$$e(\rho) = \frac{1}{2}\lambda_{ijkl}\rho(\varepsilon_{kl} - \varepsilon_{kl}^{\circ})(\varepsilon_{ij} - \varepsilon_{ij}^{\circ})$$

the elastic constant — the elastic strain

Finally, to track the microstructure evolution we just need to solve the phase field kinetic equations namely,

$$\frac{\partial\rho}{\partial t} = \nabla\cdot\left(D\nabla\frac{\delta F}{\delta\rho}\right)$$

the Diffusion coefficient

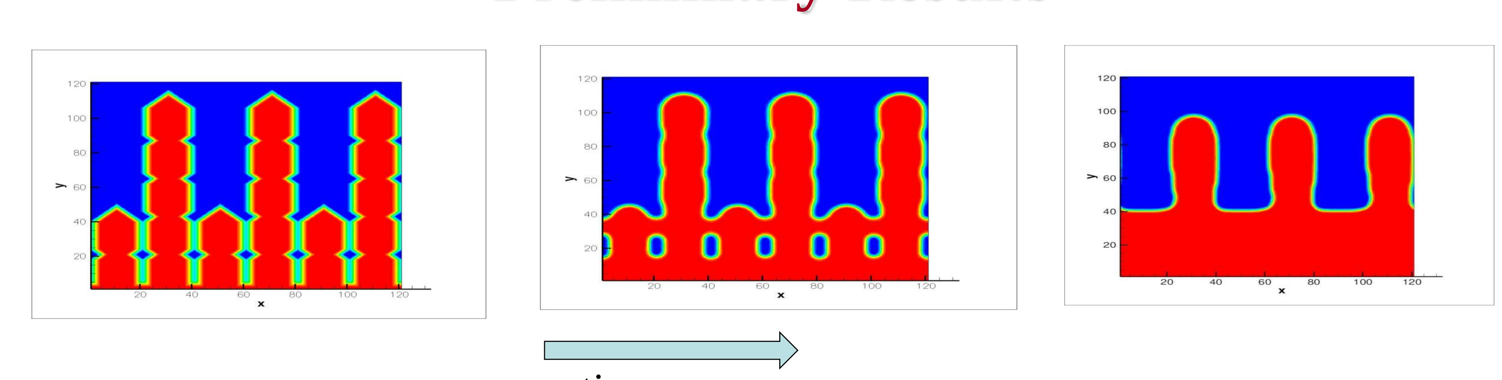
$$D = D_{surf}\rho(1-\rho) + D_{gb}\sum_\alpha\sum_{\alpha'\neq\alpha}\eta_\alpha\eta_{\alpha'} + D_{vol}\rho^3(10-15\rho+6\rho^2)$$

$$\frac{\partial\eta_\alpha}{\partial t} = -L\frac{\delta F}{\delta\eta_\alpha}$$

Numerical scheme and initial configurations

While the phase field model established above is applicable for general 3D case, only 2D solutions are presented here. In developing the 2D solution, the equations are discretized using finite difference scheme in space and explicit Euler method in time. Periodic boundary condition is applied in solving the elastic problem. The initial configurations are created to represent the actual columnar structure of the TBC produced by electron-beam physical vapor deposition (EBPVD).

Preliminary Results

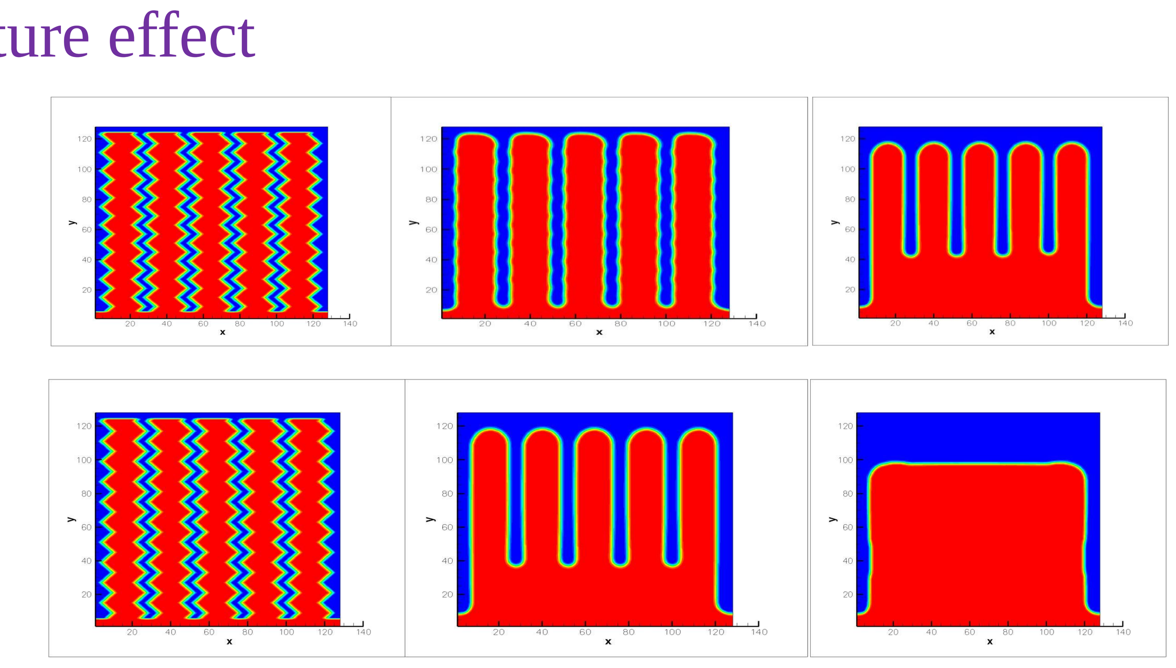


time

The feathery (Saw-tooth) structure smooth out very fast and the necks form between the columns then the material continue to transport from the top to bottom faster.

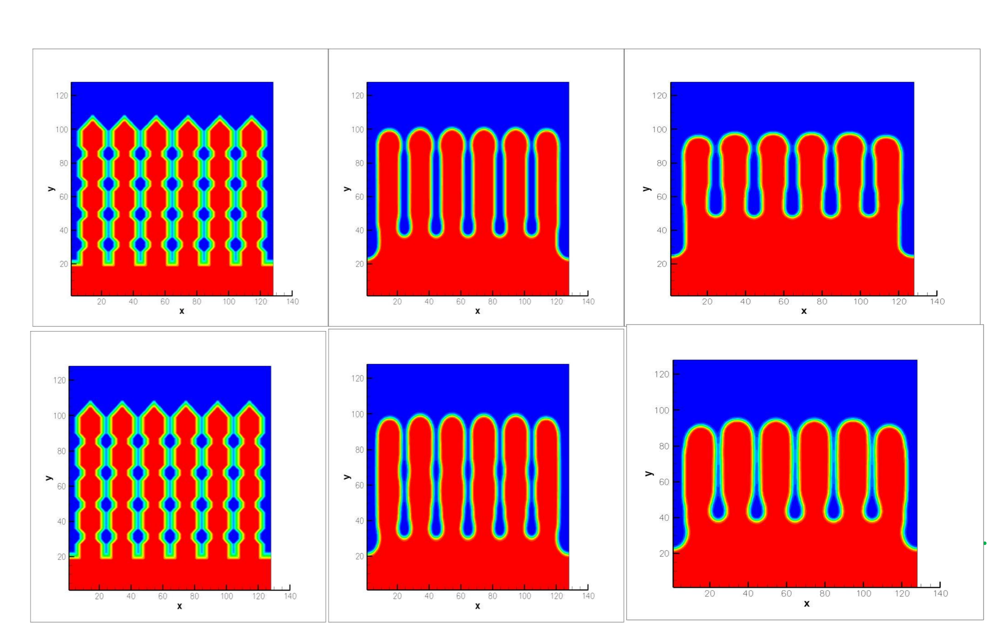
The so-called Zig-Zag structure (below) is another TBC microstructure of interest because it has smaller thermal conductivity than the regular one. This interesting microstructure can be produced by rotating the substrate during the deposition.

Temperature effect



(higher temperature)

Strain effect



(0.01 tensile strain)

Conclusion

Sintering process is mainly driven by surface and grain-boundary diffusion. So as the temperature increases, the sintering rate increases.

Mismatch strain tends to decrease the sintering rate , or in another words, constrained sintering is slower than free sintering.