Use of Covalently-Bonded Ceramics in Jet Engine Thermal Barrier Coatings
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Thin ceramic coatings are used to protect turbine blades from heat and corrosion. The protection afforded by these "Thermal Barrier Coating" (TBC) films permits greater power and fuel efficiency. Current coatings fail after repeated use. It is hoped that materials modifications to TBCs that enhance open-shell bonding at the interfaces will limit the materials failure mechanisms that currently plague TBCs.

Methodology: We have characterized atomic-level interactions at ideal TBC interfaces using a first principles density functional method. We found that interfaces with alumina, which is the typical oxidation product in current TBCs, exhibit weak adhesion.\textsuperscript{1,2,3} We postulated that one cause of the observed void formation at such interfaces is the highly ionic bonding in alumina leading to closed-shell repulsions with the nickel metal alloy. We demonstrated how doping the ceramic-metal interface with early transition metals increases local bonding and decreases closed-shell repulsions.\textsuperscript{4,5} More recently, we have investigated the effect of limiting closed-shell electronic structure at the interface by replacing alumina with a more covalently bonded ceramic, silica. We found the ideal ceramic/metal and ceramic/ceramic TBC interfaces formed using silica in place of alumina permit much stronger interface adhesion. It is hoped that materials modifications to TBCs that enhance open-shell bonding at the interfaces will limit the materials failure mechanisms that currently plague TBCs.

References:

Figure 1. A schematic view tracing how the atomic-level interfacial interactions of the TBC influence the jet engine and ultimately aircraft performance and efficiency.
Figure 2. Periodic supercell displaying relaxed atomic coordinates of a zirconia, ZrO₂, coating on silica, SiO₂. ZrO₂ serves as the outermost thermal protective layer in a TBC, and SiO₂ may be a preferred oxidation product of the metal alloy for TBC applications. The red, orange, and blue spheres represent oxygen, silicon, and zirconium, respectively. The ZrO₂ film experiences a partial phase transition upon relaxation, which agrees with previous observations and predictions for ZrO₂ thin films.