A Discrete Element Model (DEM) for Fracture Toughness of Rough Interfaces

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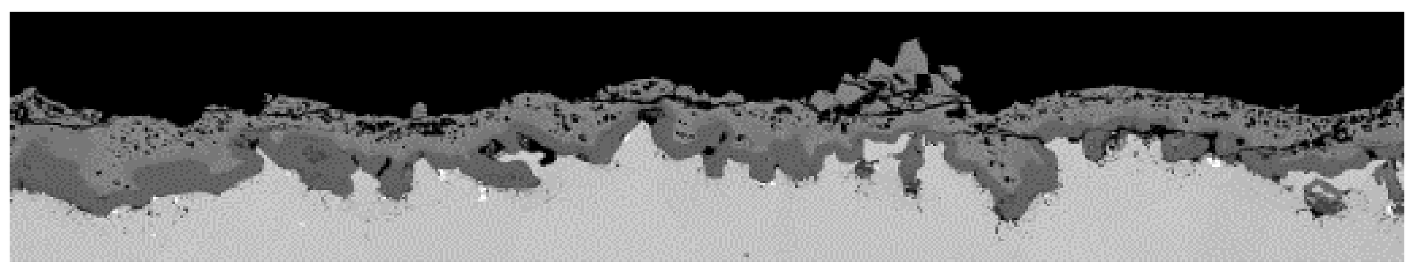
OVERVIEW

Long term mechanical reliability of SOFCs requires the multiple interfaces between dissimilar cell materials to remain fully bonded. The surface roughness of materials can be modified to improve interfacial adhesion and mechanical integrity, but the degree of improvement and dependence on material properties is not well understood. A DEM model was developed for better understanding.



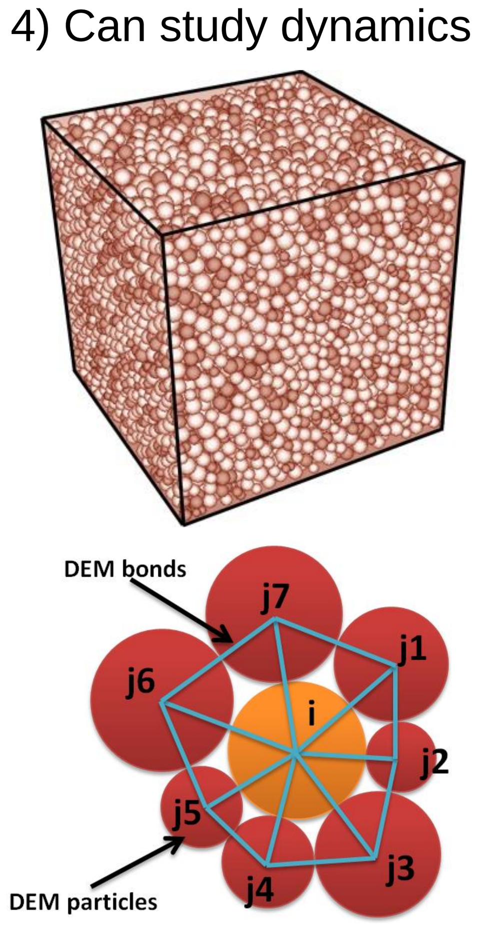
Numerical modeling in the literature shows an increasing toughness with the roughness. Experimental testing of coated metallic interconnects shows improved lifetime from surface roughness modifications. Some issues still need to be resolved:

1) Possible failure extending into the material layers;
2) Effect of relative material properties on the enhancement;
3) Optimal roughness.

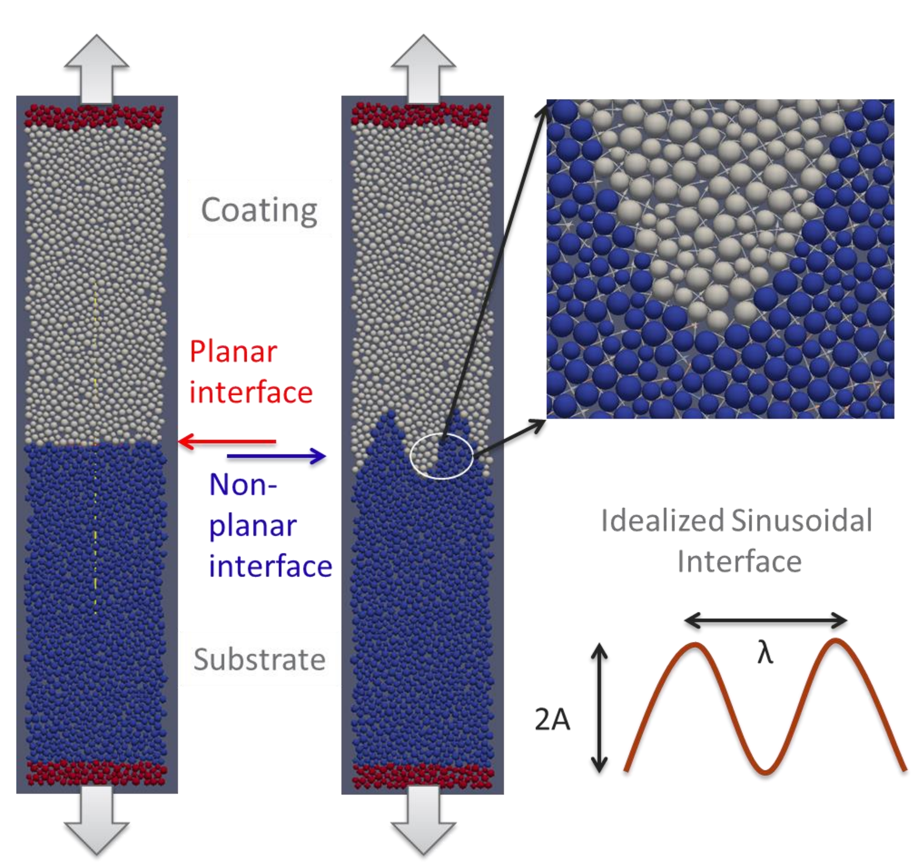
TECHNICAL APPROACH and MODEL

A discrete element model (DEM) has been developed to quantitatively simulate the interfacial delamination along the rough interface between substrate and coating materials. In the DEM model, two types of particles are used to represent the coating and substrate materials that contain an interface between them, and the body is subject to external tensile loading. The effect of interface geometry on the enhancement of fracture toughness is systematically investigated by varying the geometry of an idealized sinusoidal interface. The DEM represents a body as a packed array of bonded particles:

1) Can have random particle size;
2) Particles interact via bonds and friction;
3) Can assign material failure as a function of shear and normal stress;
4) Can study dynamics of failure propagation.



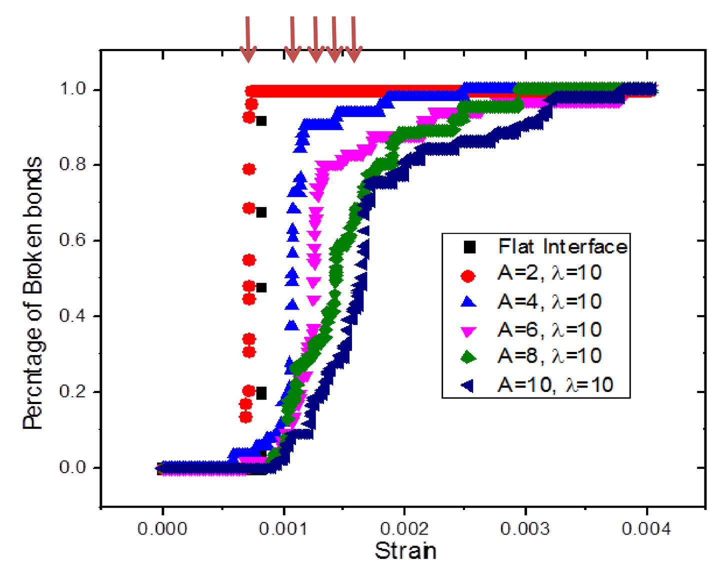
DEM particles and particle interactions



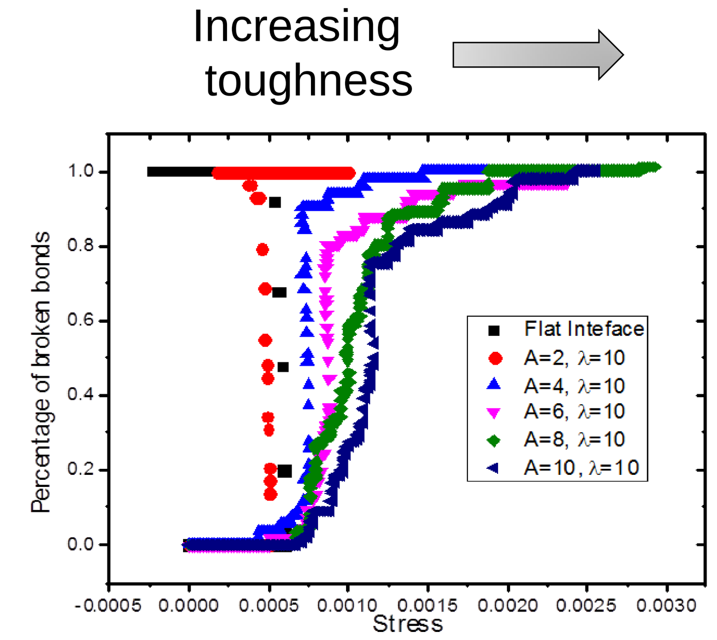
2D DEM model set up for interfaces with varying idealized roughness in terms of A/λ subject to constant strain rate loading

IDENTIFYING THE TOUGHNESS

The results curve for fraction of broken bonds at the interface versus remote applied strain exhibits an instability point that indicates the relative fracture toughness of the interface



Increasing toughness



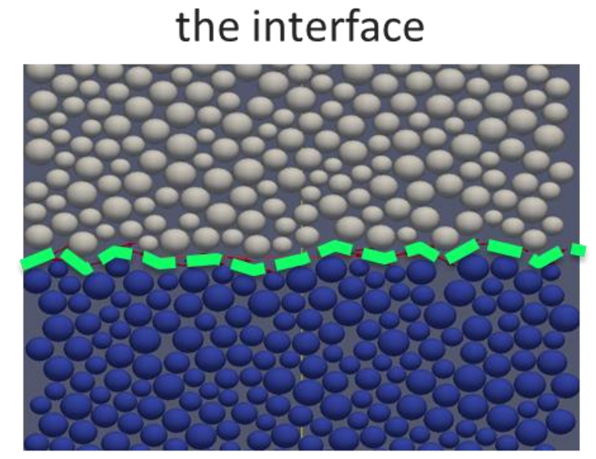
With failure permitted only along the interface, the load carrying capacity continues to increase due to mechanical interlocking between the elastic coating and substrate layers

EFFECTS OF ROUGHNESS AND MATERIAL PROPERTIES

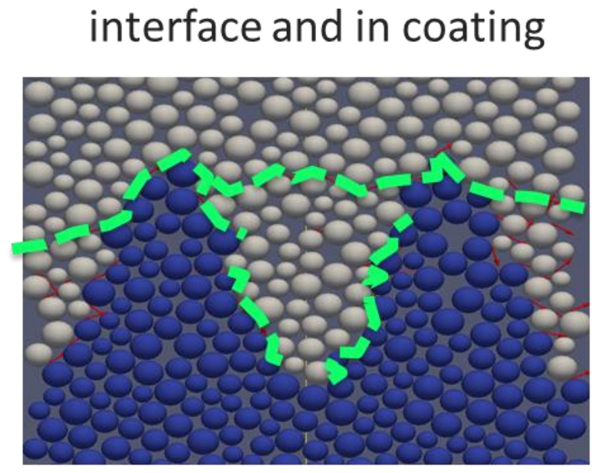
The interface toughness for different roughness is computed with models of varying interface geometry. The effect of different relative strengths of the coating layer and the interface is also studied. Different failure modes were observed for relatively weak and strong interfaces.

Weak Interfaces

Fracture occurs only along the interface

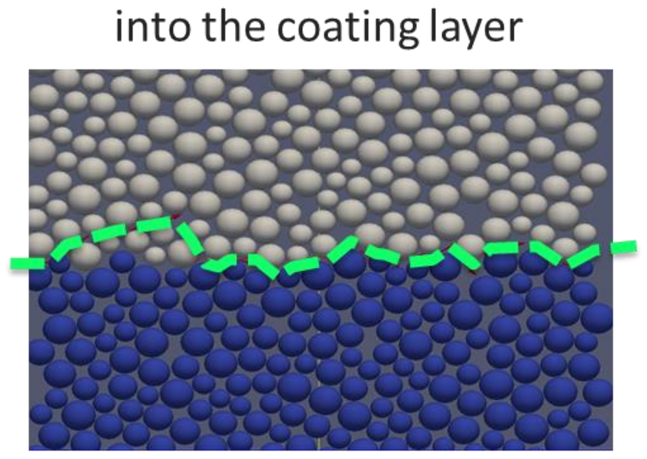


Fracture occurs along the interface and in coating

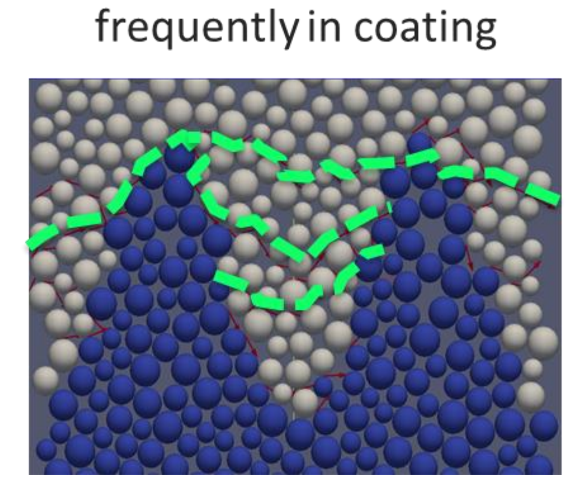


Strong Interfaces

Fracture occasionally deviates into the coating layer



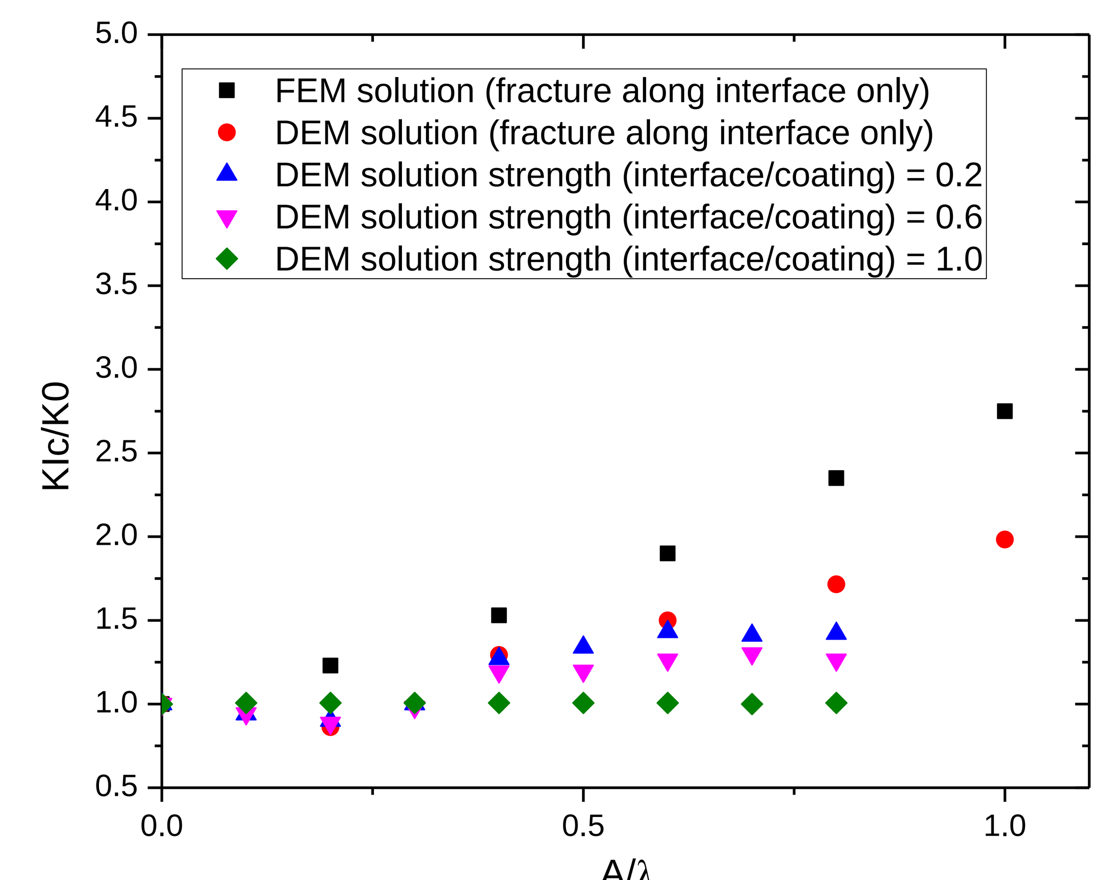
Fracture occurs more frequently in coating



Material Properties Used for the Calculations (Values Normalized by the Young's Modulus)

Property	Coating	Interface		Substrate
Young's Modulus	1.0 (250GPa)	Strong	Weak	0.8
Ultimate Strength (normal)	0.0015	0.001	0.0003	0.002
Ultimate Strength (shear)	0.001 (0.000756 – 0.0014)	0.0067	0.0002	0.0012

Increasing the roughness in general increases the relative interfacial toughness. This effect of enhancement is limited though if the interface is strong compared to the coating layer.



CONCLUSIONS

- DEM simulations can be used to both qualitatively and quantitatively model the relative interfacial toughness between two materials.
- Predicted interface strength increased due to surface roughness.
- Strengthening due to mechanical interlocking was observed.
- Failure at the interface only and/or through the material layers can be modeled.
- Failure inside the coating layer essentially limits the enhancement of interface toughness from the roughness.

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