PPPL PRINCETON PLASMA PHYSICS LABORATORY

Colloquium

Origins of Failure in Thermal Barrier Coatings from First Principles

DR. EMILY A. CARTER

Department of Mechanical and Aerospace Engineering and
Program in Applied and Computational Mathematics
Princeton University, Princeton, NJ

Aircraft engine components are protected by a multilayer, multi- component thermal barrier coating (TBC), consisting of a NiAl-based alloy layer onto which is deposited yttria-stabilized zirconia. A layer of alumina grows in between these two materials during zirconia deposition which thickens during engine use. Current TBCs fail after ~16,000 hrs of thermal cycling. In order to extend engine service lifetime, it is critical to understand mechanisms of failure and then to design circumvention strategies. We present results of first principles quantum mechanics, specifically periodic density functional theory (DFT), calculations that are used to test hypotheses about early transition metal dopants that may improve adhesion of the metal-ceramic interface, exploiting our understanding of the atomic scale origins of the weak interfacial adhesion. We also report on aspects of high temperature evolution of TBCs, including how sulfur impurities and Pt and Hf dopants may affect TBC lifetimes.

Wednesday, January 10, 2007

4:15 P.M. (Refreshments at 4:00 P.M.)

Lyman Spitzer Building, M. B. Gottlieb Auditorium