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Oxygen-poor phase observed during plasma-sprayed physical vapor deposition of zirconia coatings BRIAN GOOD, BRYAN HARDER, NASA Glenn Research Center — When cubic zirconia is deposited using Plasma Spray-Physical Vapor Deposition (PS-PVD) under oxygen-poor conditions, a metastable phase is observed. We describe a combined experimental and computational approach aimed at determining the structure and composition of the phase. X-Ray analysis indicates that the phase exhibits cubic symmetry, and it is also found to be electrically conductive, in contrast to cubic zirconia, which is electrically insulating. We have performed electronic structure calculations aimed at identifying the metastable phase. Three cubic candidate ZrO structures were identified, and the lattice constants were optimized for each. The lowest-energy structure was found to be the NaCl structure. Projected density of states calculations show that the material is conductive, with conduction occurring within the Zr 4s band. Potential technological uses for the phase are discussed.

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