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Concepts for toughening of brittle films by compositional, grain-boundary and interface design

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An enhancement of fracture toughness of hard nanostructured materials without compromising the strength is challenging as the ability of most hard materials to deform inelastically is rather limited. In this work, various innovative design strategies for fracture toughness enhancement of brittle materials will be presented, which rely on compositional, microstructure and mechanical property depth-distributions and dedicated grain-boundary and interface design. An example of the development of films with dedicated mechanical properties by a cross-sectional combinatorial approach will be given for a graded TiAlN system exhibiting variations of hardness and fracture toughness with the Al content. Another strategy for fracture toughness enhancement is a combination of hard and elastic constituents in a multilayer structure resulting in crack deflection and possible crack arrest at the interfaces. This approach will be demonstrated for TiN/SiO_x and CrN/Cr multilayer systems with various architecture. Furthermore, in order to turn catastrophic brittle fracture into a controllable deformation process, columnar grains of polycrystalline brittle TiN films were repeatedly tilted with a zig-zag fashion, which enabled multiple crack deflection accompanied by an increase of fracture toughness exceeding the values of their monolithic counterparts with columnar microstructure by more than 150%. Further fracture toughness enhancement of the sculptured films was realized through an implementation of additional interfaces by incorporating layers well differing in their structure and mechanical properties. Crack deflection along kinks of the tilted TiN columnar grains and at the elastic SiO_x interfaces was monitored in-situ by TEM revealing the role of weak grain boundaries and interfaces as effective toughening elements in analogous heterogeneous structures.
Based on these findings and results of micromechanical testing of complex multi-layered CrMnFe-based alloys varying in grain size and grain boundary network, design rules for strong and simultaneously tough structures could be established. The results will demonstrate that a dedicated compositional, grain-boundary and interface design offers great potential for the development of novel hard fracture resistant materials.

Keywords
grain-boundary and interface design