

Modification of Grain Boundary and Interfacial Structure in Al₂O₃ Coatings

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Alumina is one of the key abrasive materials for metal-cutting manufacture and semiconductor. It is also a very important thermal barrier coating in the engine system. It is known that interfaces and the mobility of atoms within an interface play pivotal role in determining the processing and properties of virtually all materials. However, the highly complex nature of the interfaces in solids has been an on-going challenge to link material performance within the internal/intrinsic interface structure and correlated atomic transport mechanism. To enhance the performance of the conventional alumina coating and meet the needs for high performance and high speed cutting applications, deliberate tuning of the grains, grain boundary and interfacial structure/chemistry are desired, those modifications would lead into the kinetic engineering and promotes oxidation, creep and abrasive resistance.

The alumina CVD coating is doped with transitional metal zirconium. The interface, referring to grain boundary as well, formed alumina and/or doped alumina grain will be modified. Thus, the performance of the resulting CVD coatings will be improved. Based on the proposed complexion interface concepts, the interface in the grain boundary is complexed and challenged to be predicted. However, thanks to the unique feature provided by advanced CVD process, the introduction and optimize the processing conditions can be precisely controlled. Therefore, both thermodynamic and growth kinetics of alumina can be well controlled. At the same time, the grain boundary relationship between doped alumina grains will be finely tuned, thus those modifications will contribute to the ultimate material performance.

The previous research showed that dopant, such as Ti, can modify the surface energy of formed oxide crystalline planes[1]. One good support on this hypothesis and practice is that the Ti-doped CeO₂ particles are showing round shape in contrast to the un-doped CeO₂ having polyhedron crystal structure. Based on the XRD analysis, it is revealed that the doped-alumina will have different texture structure comparing with corundum alumina. We calculated the texture coefficient of doped-alumina in the different crystal orientations, it is revealed that the doped-alumina will possess altering texture structure. HRTEM study suggested the dopant atoms substitution for aluminium atoms in the formed coatings. The doping process of alumina will modify not only the texture but also the atomic structure of formed grains. High resolution scanning transmission electron microscopy analyses evident that the dopant atoms may distribute at single atom level in the oxide metal ion column by substituting for aluminium ion and enriching at the grain boundary [2,3,4]. The advanced electron microscopy characterization strongly supports that dopant atoms would substitute for the aluminium atoms. Simultaneously, the dopant atoms can segregate and enrich at the grain boundary. The grain boundary engineering can provide enhanced grain interaction and dopant atoms can function as the pinning atoms or provide pinning effect for grain boundary, leading to enhancement of the thermomechanical properties. During the CVD process, the dopant atoms can be introduced into the reactor with alumina grain formations. Therefore, the atom rearrangement and mobility should be more preferable due to the vapor phase of reactants and the reduced energy. It is already accepted that the dopants will markedly strengthen the alpha-Al₂O₃ interface against mechanical deformation[5].

References:

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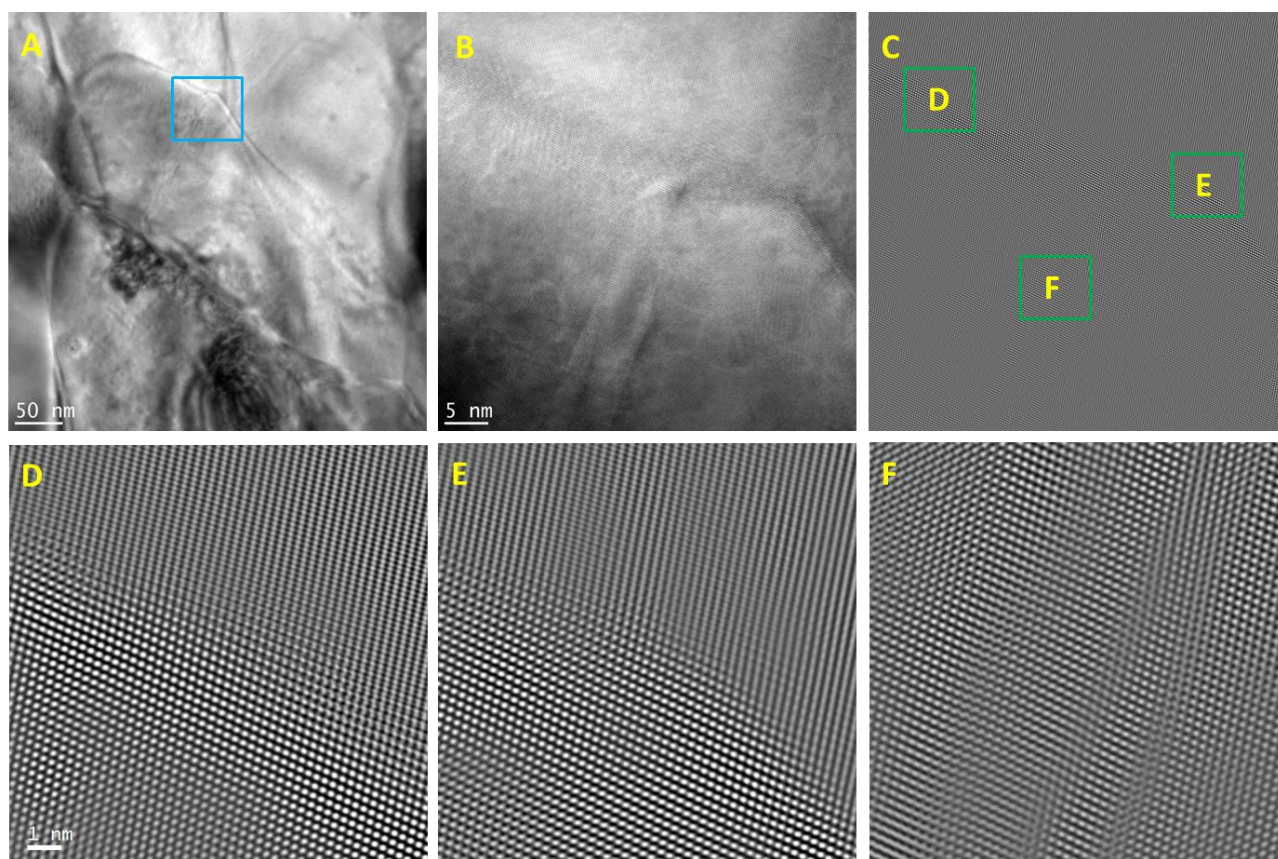


Figure 1. TEM/HRTEM images of CVD Al_2O_3 grain boundary. (A-B) TEM/HRTEM; (C) Inverse Fourier Transform filtered image; (D-E) IFT filtered images for selected areas in ; (F) IFT filtered image in C, showing the stacking faulty microstructure.