First-principles calculations of mechanical properties of aluminum oxycarbide Al_2OC

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Abstract:

Al_2OC-based intergranular layers will form in SiC polycrystals when processed with Al, B, and C additives (ABC–SiC). Various mechanical tests on hot presses ABC-SiC implied a profound influence of the interface layers on mechanical performance at ambient and elevated temperatures. However, because of the 1 nm thickness of the Al_2OC intergranular layers, experimental determination of their mechanical properties is difficult. In this study, the mechanical properties of Al_2OC were computed from first-principles and compared with those of 2H-SiC.

The crystal structure of Al_2OC is based on the hexagonal wurtzite structure. An ordered structure model was adopted. The calculations were performed using local density functional theory. Structural optimization and mechanical properties were calculated. The bulk modulus, Young's modulus and theoretical strength in [001] direction of Al_2OC and of 2H-SiC were calculated. The theoretical strength of Al_2OC was found to be about one half of that of SiC. This may provide an explanation for the improved toughness of the ABC- SiC samples, as a consequence of fracture propagating along the weaker Al_2OC grain boundary films.