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THE ANISOTROPY OF THERMAL CONDUCTIVITY IN DIBORIDES OF ZIRCONIUM AND HAFNIUM

Abstract

Diborides of zirconium and hafnium based ultra high temperature ceramics have been widely used as non-ablative thermal protection materials. The elastic anisotropy plays an important role in their thermal conductivity behavior. In this paper, the anisotropic elastic and thermal properties of layered ZrB2 and HfB2 with the AlB2 structure have been investigated by from first principles using density functional theory in a wide temperature ranges. The factors determining the significance in anisotropy in AlB2-type diborides are discussed from crystal structure and atomic bonding characters. For instance, the calculated in-plane thermal conductivity is always larger than that along the c-axis, parallel to the layer stacking direction.