Abstract Guide

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Modeling and Experimental Conditions of Bulk Silicon Carbide Growth

T.A. Bowen, Y.K Shin, Y. Xuan, A.C.T. van Duin, and J.A. Robinson

Silicon carbide (SiC) growth and research, long dominated by industry, is now being reintegrated into U.S. academic institutions. The Silicon Carbide Innovation Alliance (SCIA), supported by initial funding from Onsemi and the Air Force Office of Scientific Research, is spearheading this effort by establishing a state-of-the-art growth center. Equipped with advanced furnaces, SCIA is rapidly advancing in the production of 6-inch SiC wafers. The center has already demonstrated its capability by successfully growing several boules, which are being processed into crystallographically aligned pucks and diced into wafers for further defect characterization.

The growth of bulk SiC boules is a complex process that demands a strong theoretical foundation to guide extensive experiments and accelerate progress in the field. To this end, computational modeling and simulations are employed to accurately describe the solid-phase SiC, sublimation processes, and the resulting SiC vapor species as a function of temperature. This computational approach utilizes atomistic models at the nanoscale, specifically employing the ReaxFF reactive force field. Data derived from second-order Møller-Plesset perturbation theory (MP2) indicates that large clusters, such as Si_2C_3 and Si_2C_2, are the predominant sublimated species in the temperature range relevant to our growth processes. Understanding these physiochemical details of SiC evaporation allows us to enhance computational fluid dynamics (CFD) models by incorporating more accurate chemical descriptions, thereby improving the overall growth process.

Experiments are being conducted with various felt materials and configurations to assess the impact of hot zone design on the heat flow during SiC growth and its subsequent effect on the quality of the final product. The underlying hypothesis is that more efficient heat trapping within the growth system will result in higher quality SiC boules.