HPHT Growth and Modeling of High-quality Defect-free Diamond Crystals

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1. Introduction

Diamond substrates for next-generation quantum computation/metrology, power electronics, and X-ray optics applications require high-crystallinity crystals with minimal defects density. We developed the modified High-Pressure High-Temperature (HPHT) temperature gradient growth technology that allows growing the highest crystalline quality large diamond crystals with a dislocation density of fewer than 10^0 cm^{-2}. This near-equilibrium process is carried out under extreme conditions, where diamond single crystals are grown from a carbon solution in molten metal solvent (Fe, Ni, and Co and their alloys) under pressures in excess of 5 GPa and temperatures of 1,600 K and higher. Since there are no available diagnostics to directly monitor crystal growth in the HPHT cell, both indirect experimental growth monitoring and faithful models are needed to connect experimental outcomes to system design and process conditions. We present results from a collaboration that includes experimental growth carried out at the Euclid Beamlabs, two modeling efforts by the University of Minnesota and Fraunhofer IISB, and X-ray crystals characterization conducted by APS/ANL. This three-fold approach provides rigorous tools to both understand growth in this system and to perform subsequent optimization of growth conditions. In particular, we aim to more fully understand the fundamental aspects of diamond nucleation and growth and identify process conditions that will achieve the highest crystalline quality in large diamond crystals.

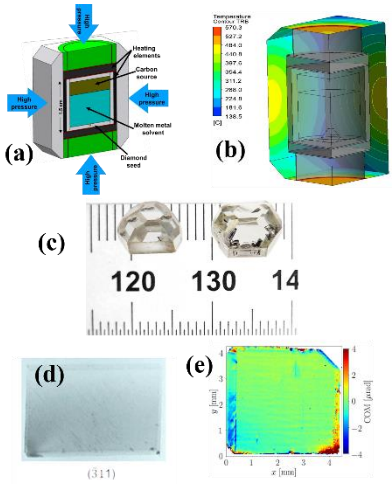

Figure 1. (a) The cross section of the inner growth chamber; (b) Combination of 3D ANSYS model for thermal field and diamond 2D axisymmetric growth model are used (Fraunhofer IISB, UMN) (c) Grown single crystal Type Iia HPHT diamonds; (d) X-ray topography demonstrates dislocation-fre diamond plate; (e) Color map of center of mass (COM) of Bragg reflection angular dependencies of diamond plate with extremely small average arms= 0.12 µrad.

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