Understanding Transport and Kinetic Effects during High-Pressure, High-Temperature (HPHT) Growth of Single-Crystal Diamond

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Diamond single crystals are of great interest for future applications in high-power, X-ray optical elements, power electronics, and quantum computing devices, and the demand for high-quality, lab-grown diamonds is expected to grow dramatically. The High-Pressure, High-Temperature (HPHT) process is capable of growing diamond single crystals, of centimeter size and with dislocation densities less than 10 cm^{-2}, from a molten metallic solvent under pressures of 5 GPa (50,000 atmospheres) and temperatures of 1,500 K and higher.

These severe conditions make *in situ* diagnostics impossible, so we have developed a multi-scale, continuum-level computational model to probe the mechanistic underpinnings of HPHT diamond growth. This model is the first to rigorously connect carbon transport through the solvent to phase-change kinetics of growth along the faceted crystal [1]. Analyses will illustrate the importance of flow, carbon transport, and temperature distributions on growth rate, which favorably compare to experimental data [2]. Results also demonstrate how inhomogeneities in supersaturation arise along the crystal facets as crystal size increases, and we discuss how this effect may lead to inclusion formation–defects that must be avoided for high-quality crystals.

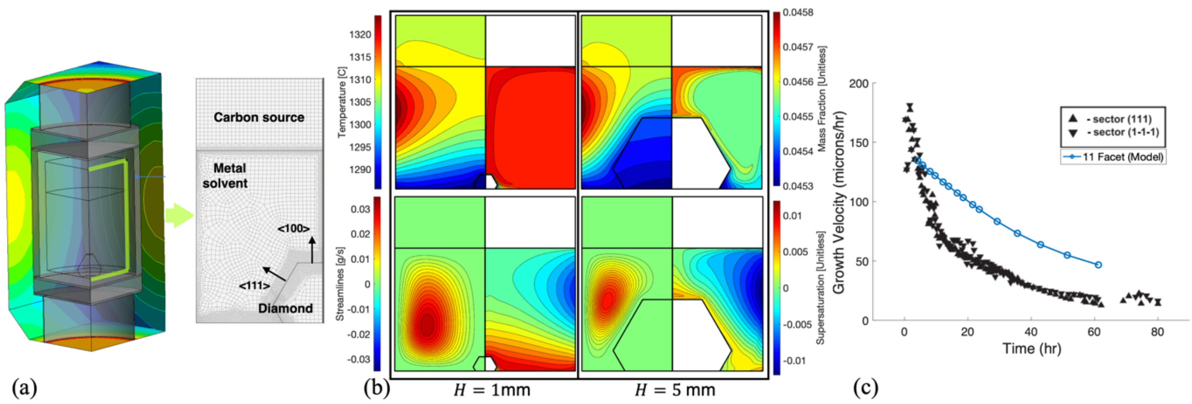

Figure 1: (a) Our model represents 3D heating of the growth cell (left), which then informs a 2D analysis of solvent flow, carbon transport, heat transfer, and growth (right). (b) Example calculations are shown for crystal sizes of 1 and 5mm height. (c) Computed (model) growth rates are compared to HPHT growth data along the (111) facet [2].

References

[1] S.S. Dossa *et al*. Analysis of the High-Pressure High-Temperature (HPHT) Growth of Single Crystal Diamond. *J. Crystal Growth*. 2022. (In review)
[2] Y.V. Babich *et al.* Nitrogen aggregation and linear growth rate in HPHT synthetic diamonds. *Diamond and Related Materials.* 2004; **13**: 1802-1806.
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