Elmer Simulations in Kyropoulos Sapphire Crystal Growth

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Objectives

- Elmer simulations are separately made for physical mechanisms present in KY sapphire crystal growth, and include the following cases:
  - Case1: Heat transfer by conduction and radiation in/between solid materials
  - Case2: Automatically adjusted heater power to balance the melting temperature at 3-point
  - Case3: Search for the shape of the crystal-melt interface during steady-state growth
  - Case4: Sapphire melt flow induced by Marangoni and Grashof convections coupled with conduction and radiation in/between solid materials and melt

Geometrical Details

- Typical KY geometry (see below)
- Simplifications:
  - Heater contains single blocks in horizontal and vertical sections (*)
  - Radiation (molybdenum) shields are considered as single blocks (**)

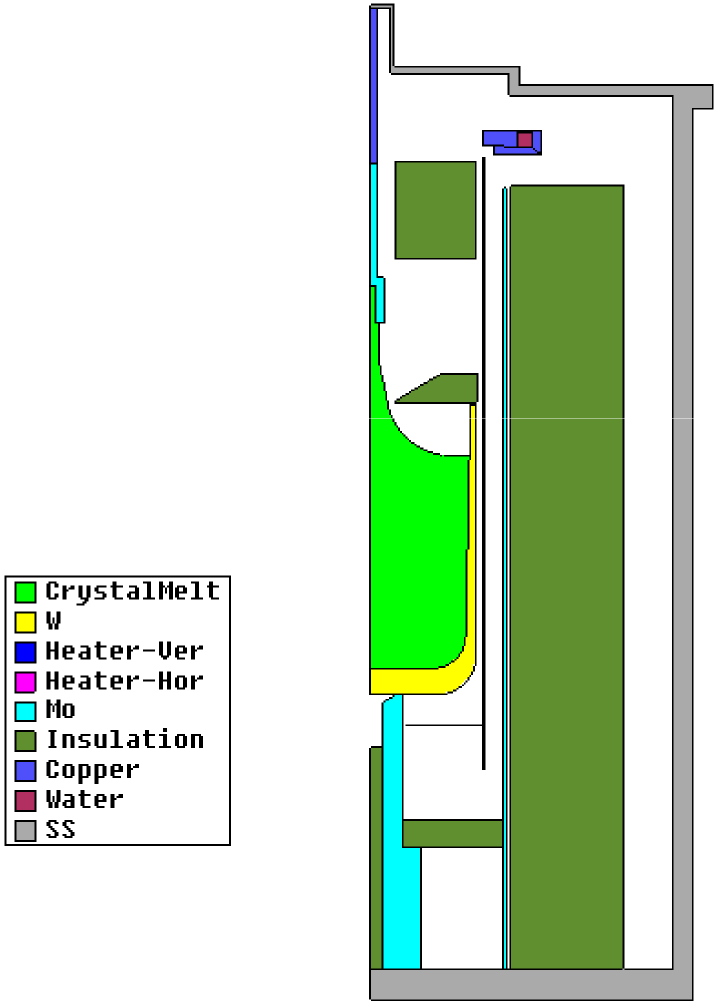
(*) Elmer has no limitations to model multi-block heater sections
(**) In Elmer, real axi-symmetric ('volumetric') Mo shields have to be considered. The radiation shields may be replaced with solid single blocks with effective heat conductivities calculated from Fourier's law, see Chen et.al. Journal of Crystal Growth, 318 (2011)

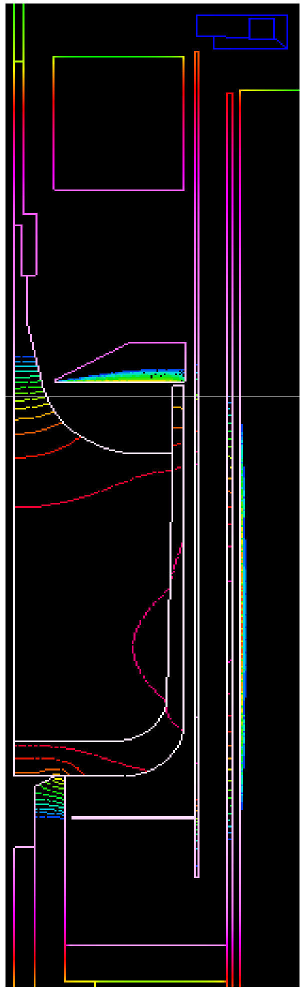
Case1: Details

- Heat transfer by conduction and radiation in/between solid materials only
- Crystal and melt considered together as a single solid block (crystal material properties)
- Constant heater power in horizontal and vertical heater sections
- Material parameters:
  - See Miyagawa et.al., Journal of Crystal Growth 402 (2014), Liu et.al., Journal of Crystal Growth 431 (2015)
  - Crystal transparency modeled with Rosseland's method (*)
- Computational mesh: Triangle element size 5mm except in horizontal/vertical heater sections and surrounding Mo-ring (3mm)

(*) Widely used in literature to replace full radiation model in transparent material, see for instance Liu et.al., "Study on crystal-melt interface shape of sapphire crystal growth by the KY method, Journal of Crystal Growth, 431 (2015)

Case1: Process Geometry and Numerical Results for Temperature Distribution





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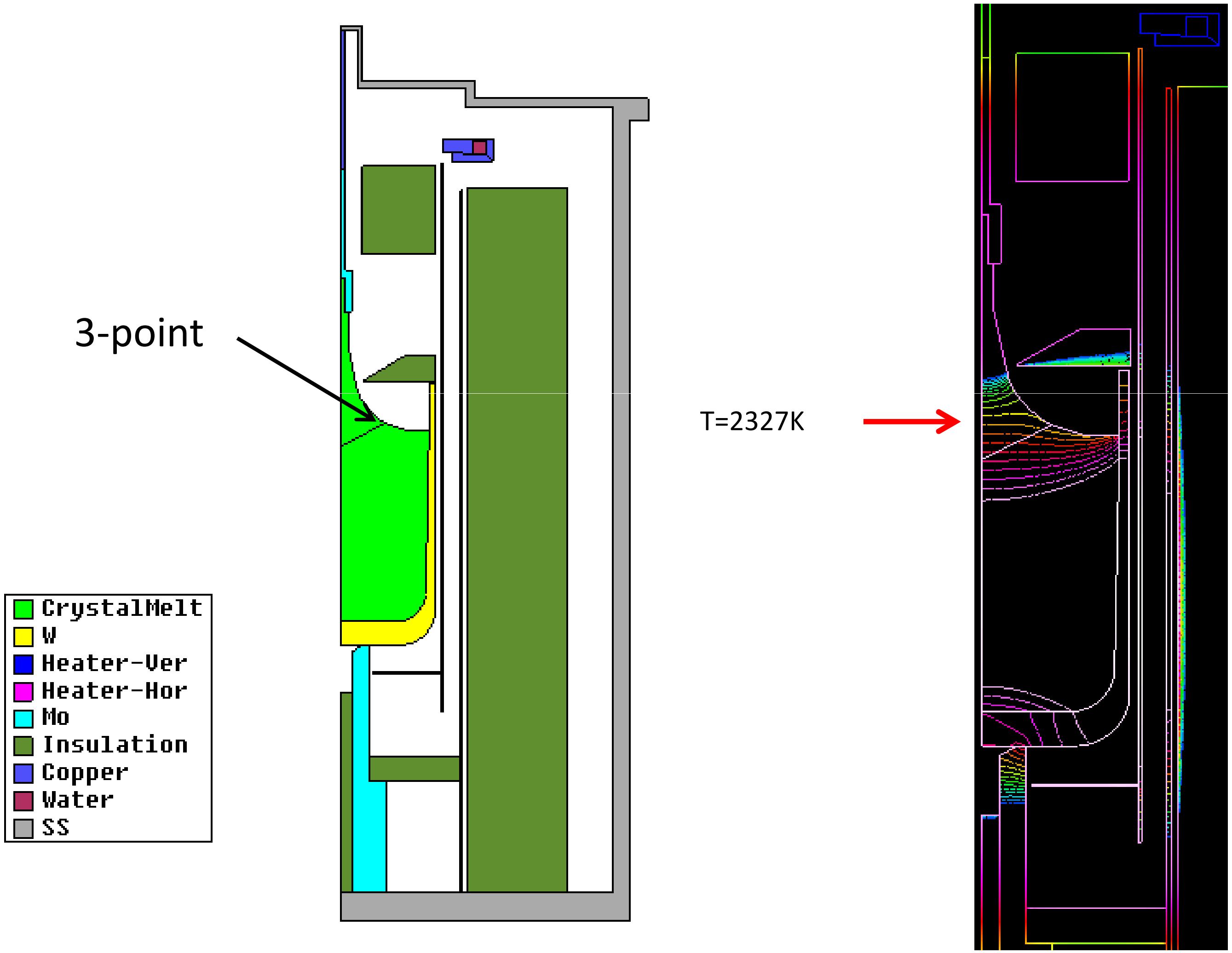
Case2: Details

- Heat transfer by conduction and radiation in/between solid materials
- Crystal and melt considered together as a single solid block (crystal material properties)
- Constant heater power in horizontal section, heater power in vertical section adjusted in such a way that T=2327K (melting point temperature) at 3-point
- Material parameters:
  - See Miyagawa et.al., Journal of Crystal Growth 402 (2014), Liu et.al., Journal of Crystal Growth 431 (2015)
  - Crystal opaque, constant heat conductivity (k=3.4 W/mK)
- Computational mesh: Triangle element size 5mm except in horizontal/vertical heater sections and surrounding Mo-ring (3mm)

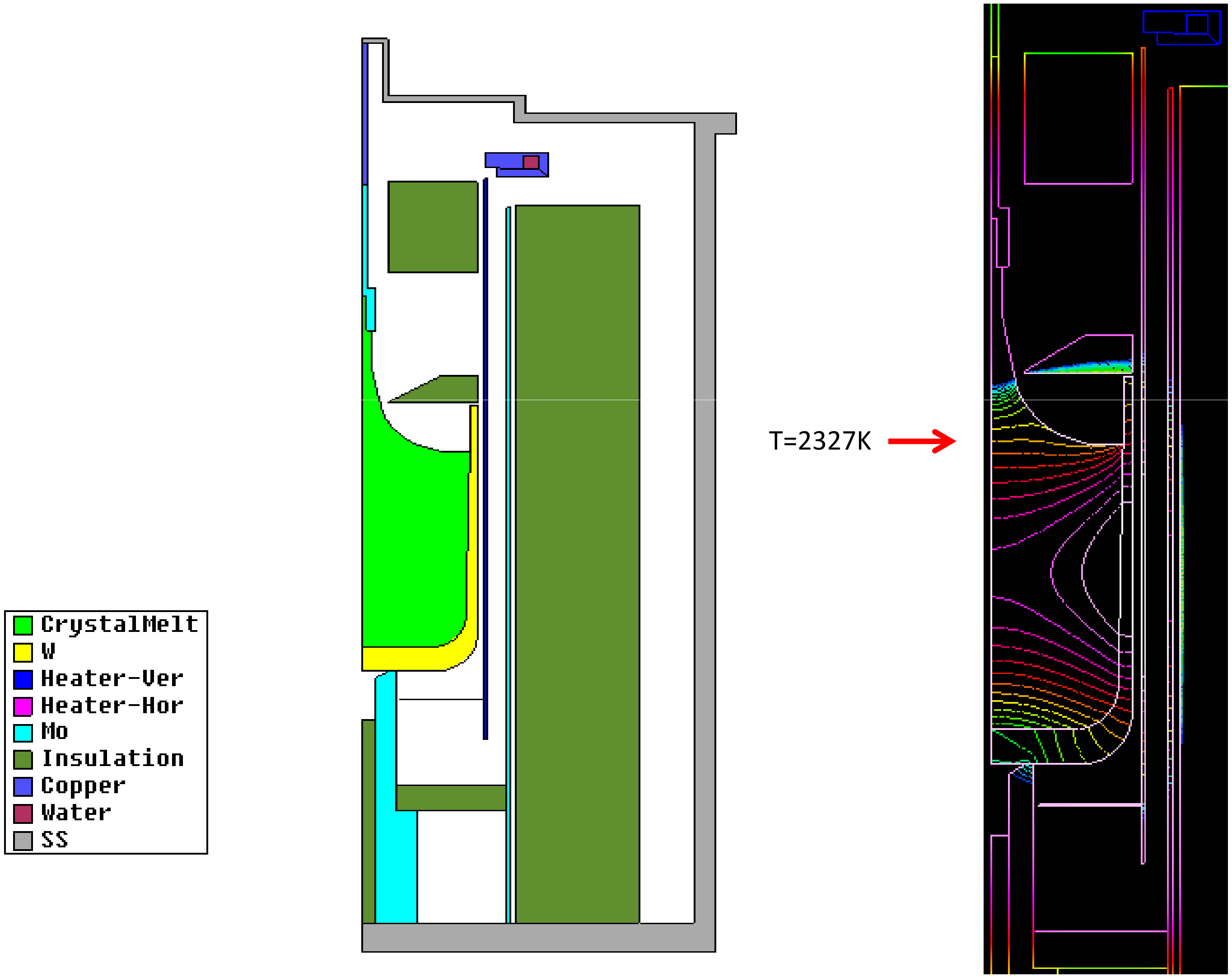
Case2: Process Geometry and Numerical Results for Temperature Distribution



Case3: Details

- Heat transfer by conduction and radiation in/between solid materials, no melt convection
- Crystal, melt and free interface present in the system (T=2327K at interface)
  - Single crystal-melt block (enthalpy method, fixed grid)
- Constant heater power in horizontal section, heater power in vertical section adjusted in such a way that T=2327K at 3-point
- Material parameters:
  - See Miyagawa et.al., Journal of Crystal Growth 402 (2014), Liu et.al., Journal of Crystal Growth 431 (2015)
  - Crystal opaque, constant heat conductivity (k=3.4 W/mK)
- Computational mesh:
  - Triangle element size 5mm except in horizontal/vertical heater sections and surrounding Mo-ring (3mm)

Case3: Process Geometry and Numerical Results for Temperature Distribution



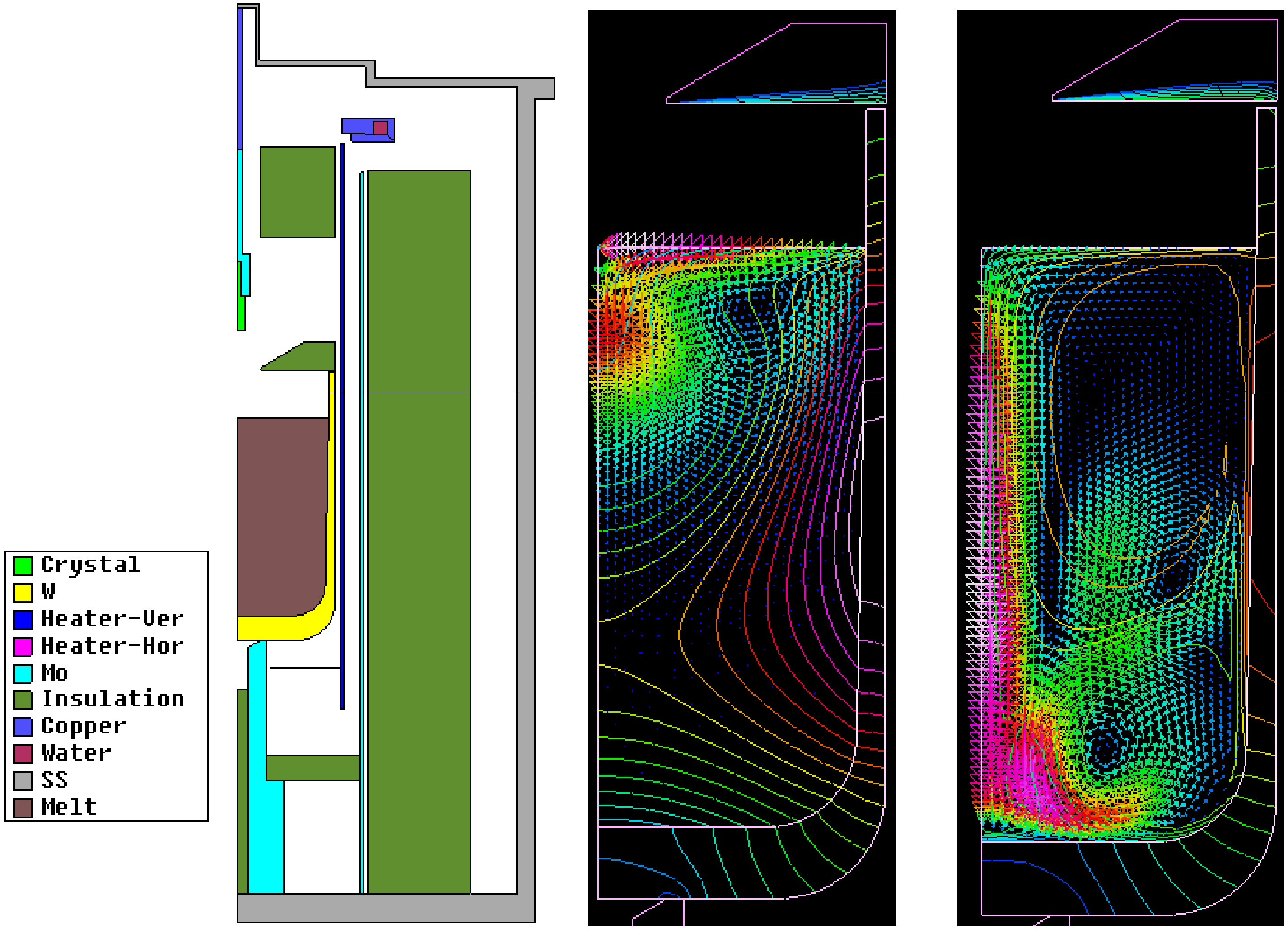
Case4.1: Details

- Just before seed-dipping (no physical contact between seed-crystal and melt)
- Heat transfer by conduction and radiation in/between solid materials and melt
- Sapphire melt flow driven by Marangoni convection
- Constant heater power in horizontal section, heater power in vertical section adjusted in such a way that T=2305K at the center of melt surface
- Material parameters:
  - See Miyagawa et.al., Journal of Crystal Growth 402 (2014), Liu et.al., Journal of Crystal Growth 431 (2015)
- Computational mesh: Triangle element size 5mm except in horizontal/vertical heater sections and surrounding Mo-ring (3mm)

Case4.2: Details

- Just before seed-dipping (no physical contact between seed-crystal and melt)
- Heat transfer by conduction and radiation in/between solid materials and melt
- Sapphire melt flow driven by Grashof convection
- Constant heater power in horizontal section, heater power in vertical section adjusted in such a way that T=2305K at the center of melt surface
- Material parameters:
  - See Miyagawa et.al., Journal of Crystal Growth 402 (2014), Liu et.al., Journal of Crystal Growth 431 (2015)
- Computational mesh: Triangle element size 5mm except in horizontal/vertical heater sections and surrounding Mo-ring (3mm)

Case4: Process Geometry and Numerical Results for Temperature Distribution and Velocity Field



Numerical results: Marangoni convection (left), Grashof convection (right)

Conclusions

- In Elmer simulations, a simplified geometry and material parameters have been used to realize Elmer capabilities in solving KY sapphire crystal growth
  - Elmer shows consistent results compared to a well-known commercial crystal growth software in heat transfer, crystal-melt interface shape and melt flow when separately tested
    - The differencies are – 0.5% in temperature distribution (maximum temperature), -1.0% in adjusted heater power, and -5.0% in velocity field (maximum velocity)
  - Tracking of crystal-melt interface is based on enthalpy method, which allows the analysis of 'sugaring' in the remaining melt in the bottom of the crucible
  - Elmer does not include a routine to simulate radiation in transparent solid material; this property has been replaced with Rosseland's method widely used in the literature

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Overall Remarks

- Elmer capabilities in crystal growth are not limited to the physical cases presented in this analysis, but also includes
  - Thermal stresses in crystal
  - Transportation of species (e.g., particle drifting in melt)
  - Transient and 3D analyses
- Elmer allows unlimited parallel simulations and multiple single-processor simulations simultanously
- Elmer is an open-source without any (annual) license fees