Optimization and Control of Aluminum Nitride Crystal Growth

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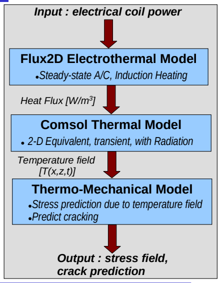
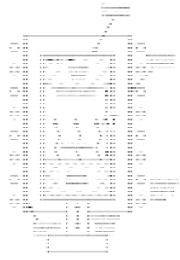
Project Overview

- Modeling electromagnetic + thermal + mechanical physics of crystal growth
- Project goals : (1) reduce cracking due to thermally-induced stress during cooldown; (2) improved thermal control for better crystal quality
- Use thermo-mechanical crystal models to predict stress and cracking from applied temperature
- Use feedback control and estimation to maintain desired conditions for optimal growth



Crystal Growth Process

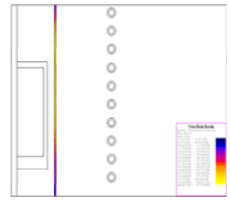
- Crystal grown in induction furnace at high temperature (>2250 C)
- Sublimation-deposition process evaporates source material, condenses to form crystal
- Three distinct growth phases : heat-up, growth, cool-down
- Strict temperature constraints to optimize crystal quality
- Unable to measure process variables directly, limited run-time feedback



Electromagnetic Model

- Flux 2D package used to solve steady-state induction heating problem
- Input : power into heater coil, output : volumetric heat flux into susceptor
- Heat flux scales linearly with input power and dynamics are very fast (assumed instantaneous)
- Output to thermal model:

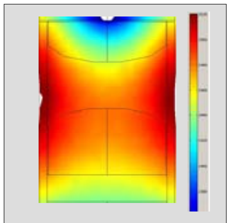
$$Q_s(z,t) = u(t)Q_{ss}(z)$$



Result : Heat Flux Data [W/m³]

FEM Thermal Model : Comsol

- Transient FEM model with all relevant thermal phenomena
- Comsol Multiphysics package integrates very well with Matlab
- Inputs : susceptor heat flux, vertical crucible position
- Model matches well to experimental data
- Ongoing work to optimize key uncertain parameters using experimental data



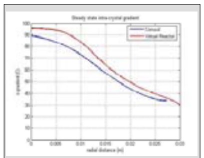
Section of growth furnace geometry showing temperature distribution, temperatures in K

FEM Model Calibration : Overview

- Use Matlab's optimization tools to adjust uncertain parameters (X) to minimize mismatch between model and experiment

$$\min_X \; J(X)$$
$$S.T. \quad X_l \le X \le X_u$$
$$J(X) = \sum_i W_1\|y_1(r,\theta,z,t)-\hat{y}(r,\theta,z,t)\|_2 + W_1\|y_1(r,\theta,z,t)-\hat{y}(r,\theta,z,t)\|_\infty + \cdots + W_i\|y_{ss}(r,\theta,z)-\hat{y}(r,\theta,z)\|_2 + W_i\|y_{ss}(r,\theta,z)-\hat{y}(r,\theta,z)\|_\infty$$

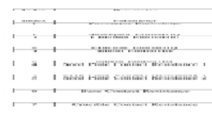
y_{ss} = temperature profile, experimental
$\hat{y}$ = temperature profile, Comsol model
W_i = optimization weightings



Result showing good agreement in intra-crystal temperature gradient at steady-state growth temperature

FEM Model Calibration

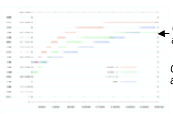
- Key parameters chosen based on physical knowledge
- Initial values from CIS. Normalized scaling factor multiplies temperature-dependent and anisotropic behavior



Thermo-Mechanical Modeling

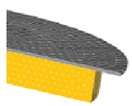
- Goals:
  - Model stress state in AlN crystal as a function of temperature field
  - Predict cracking based on stress state
- Approach:
  - Implement thermo-elastic material model for use with in-house FEM modeling software
  - Create FEM model of AlN boule
  - Apply temperature field as supplied from FEM
  - Compute resolved normal stress on critical planes in AlN crystal
  - Determine critical value for resolved normal stress based on fracture toughness

Thermo-mechanical modeling



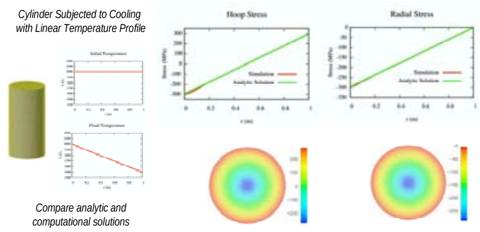
CTE as a function of temperature as implemented in modeling code

Geometry of simulated crystal and backing plate



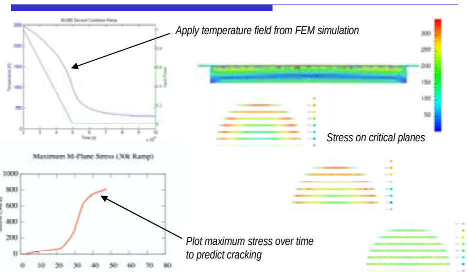
Validation Test Problem

Cylinder Subjected to Cooling with Linear Temperature Profile



Compare analytic and computational solutions

Thermo-mechanical Analysis



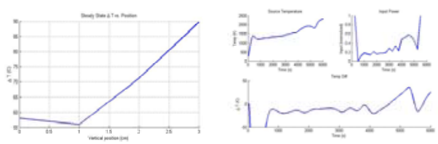
Apply temperature field from FEM simulation

Stress on critical planes

Plot maximum stress over time to predict cracking

Control : Heatup Phase

- Objective : minimize ΔT while bringing T_{source} to 2250 C
- Model-based optimization approach, no process feedback
- Available inputs : heater coil power, crucible position
- Use power input or crucible position to minimize ΔT during heat-up

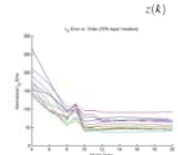


- Good control over ΔT, but need to change position and power

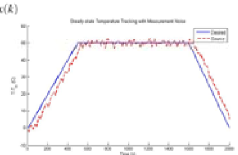
Control : Growth Phase

- Objective : regulate ΔT and T_{source} to desired values
- Identify linear model, build optimal estimator, design optimal control law

$$x(k+1) = A_m x(k) + B_m u(k) + w(k)$$
$$y(k) = C_m x(k) + v(k)$$
$$z(k) = C_z x(k)$$



L_2 error in reduced order model response



Tracking performance at growth temperature