

NanoArc RevB SAT Crystallization Route Development Plan

Chemical Nucleation, Retained Seed,
and On-Demand Trigger Screening

Project	NanoArc - Mira/Zoey/Rumi thermal development
Status	Draft experimental protocol - not approved, frozen, or implemented
Revision	Rev0
Date	2026-08-13
Scope	RevB bench development with possible later Rumi/RevC integration
Authority	Tristan retains design, safety, approval, and freeze-break authority
Relationship	Standalone companion to the RevB/RevC PCM Development Proposal

Purpose. Establish a controlled, low-equipment programme for finding a repeatable SAT crystallization mechanism without depending on unobtainable DHPD. Three routes are compared using common 5 g microcells before CMC, graphite, cartridge geometry, or ACE supervision is allowed to confound the result.

Decision principle. Automatic cooldown recovery is the primary Rumi objective. Retained-seed and commanded-trigger routes remain valid alternatives, but no route is credited until it survives complete melting, repeated cooling, and the defined acceptance gate. RevA remains unchanged.

Contents

Executive summary	2
Programme boundaries	2
Revision and ownership relationship	2
Explicit exclusions from the initial screen	2
Materials and records	2
Common apparatus and controls	3
Minimum apparatus	3
Specimen controls	3
Thermal profiles	4
Stage A - service-like screen	4
Stage B - over-temperature robustness	4
Stage C - route qualification	4
Measurements	4
Data schema	5
Common acceptance gates	5
Automatic-recovery gate	5
On-demand gate	5
Route 1 - chemical nucleators	5
Initial screen	5
Candidate interpretation	6
Optimization	6
CMC integration	6
Household candidate annex	7
Route 2 - retained SAT seed	7
Principle	7
Two-zone proof cell	7
Thermal-isolation gate	8
Route 3 - on-demand triggering	8
Shared pre-trigger condition	8
Localized cold spot	8
Mechanical snap disk	8
Down-selection	8
Safety and stop conditions	9
References and evidence status	9
Evidence labels	10
Approval and completion record	10

Executive summary

Sodium acetate trihydrate (SAT) stores substantial latent heat near 58 C, but it can remain supercooled and can separate after incongruent melting. A seed crystal introduced after cooling can trigger crystallization, yet an ordinary SAT seed dissolves during a complete melt. This plan therefore develops three independent solutions:

1. **Chemical nucleation:** add a persistent, defined crystalline material that promotes automatic crystallization.
2. **Retained SAT seed:** preserve genuine SAT trihydrate in a thermally isolated pocket while the main charge melts.
3. **On-demand trigger:** retain a supercooled charge and initiate crystallization using a localized cold spot or documented commercial snap disk.

All routes start with identical 5 g specimens and common thermal profiles. Chemical candidates are screened alone. CMC is introduced only after a nucleation route passes, because it may coat, redistribute, or inhibit the active surface. Commercial expanded graphite and the Black Donald specimen BDG-01 enter only after nucleation plus CMC is reliable; graphite is treated as a heat-transfer and containment variable, not an accepted nucleator.

This document is an executable development protocol, not a production formulation, safety certification, cartridge release, firmware specification, or authorization to alter frozen RevA hardware.

Programme boundaries

Revision and ownership relationship

- **RevB** is the prototype and characterization platform.
- **Rumi/RevC** is the possible integration target after evidence exists.
- **RevA** receives no schematic, PCB, firmware-contract, connector, or safety-policy change.
- Initial work uses a controlled dummy fixture, not the Weld Energy Stage.
- ACE-derived automation may later supervise temperature profiles, logging, sensor validity, cycle counting, and fault detection. Heater power switching and independent over-temperature protection remain fixture responsibilities.

Explicit exclusions from the initial screen

- CMC, graphite, BDG-01, metal foam, and final cartridge materials;
- combined or binary nucleators;
- homemade chemical substitutions without identity and batch records;
- pressure vessels or completely rigid sealed containers lacking rated headspace and relief engineering;
- production claims based only on literature values or a single successful cycle.

Materials and records

Formal SAT stock intake is a separate administrative gate. Use SAT_STOCK_QUALIFICATION.md to distinguish documented stock intended for SAT-0 formal cells from the household, exploratory SAT-HM-001 rehearsal. This draft route does not qualify stock and does not change the historical PCM-C identity retained in ../Proposals/NanoArc_PCM_Cartridge_PCM_Reconciliation.md.

Every material receives a supplier, product, lot, grade, CAS number, hydrate state, received date, storage condition, SDS location, and certificate-of-analysis status. A consumer product is acceptable only when its ingredient identity is sufficiently specific for the relevant experiment.

Material	Identity / CAS	Programme role	Initial status
SAT	Sodium acetate trihydrate / 6131-90-4	PCM and positive seed	Required
SS	Sodium sulfate, anhydrous / 7757-82-6	Accessible chemical nucleator	ACS material and SDS available
CaCl ₂ ·2H ₂ O	Calcium chloride dihydrate / 10035-04-8	Strong literature comparator	Source exact hydrate
MgCl ₂ ·6H ₂ O	Magnesium chloride hexahydrate / 7791-18-6	Secondary literature comparator	Source exact hydrate
TPD	Tetrasodium pyrophosphate decahydrate / 13472-36-1	Phosphate alternative	Deferred until sourced
Borax	Sodium tetraborate decahydrate / 1303-96-4	Household-accessible alternative	Verify pure decahydrate
NaCl	Sodium chloride / 7647-14-5	Household-accessible alternative	Additive-free pickling salt preferred
CMC-Na	Sodium carboxymethyl cellulose / 9004-32-4	Later separation control	Reliable grade still required

The local SDS and study library is maintained under Chemistry/SDS/ and Chemistry/References/. An SDS establishes handling identity and hazards; it does not replace a lot-specific certificate of analysis.

Common apparatus and controls

Minimum apparatus

- balance resolving at least 0.001 g;
- identical thermally rated borosilicate microcells;
- compatible closures with defined headspace and secondary containment;
- controlled bath or heater capable of 25-80 C profiles;
- one logged specimen probe per cell plus bath/heater and ambient probes;
- timer and data logger;
- camera and fixed visual-inspection background;
- labels that remain legible through heat and moisture exposure;
- independent over-temperature cutoff not dependent on experiment software.

PTFE tape may improve vapour retention around a compatible stopper, following the 2024 study approach, but it does not convert an unrated vial into a pressure vessel. Do not heat a rigid hermetic vessel unless it is explicitly rated for the pressure and temperature involved.

Specimen controls

ID	Contents	Purpose
FIX-EMPTY	Empty instrumented cell	Fixture lag and sensor sanity
SAT-0	5.000 g pure SAT	Negative control for spontaneous crystallization

ID	Contents	Purpose
SAT-SEED+	5.000 g pure SAT, manually seeded only after cooling	Positive crystallization and heat-release proxy control
ROUTE-BLANK	Route-specific geometry without active seed/trigger	Separates mechanism from geometry

Use three independently prepared cells for each condition. Do not treat three cycles in one cell as three independent specimens.

Thermal profiles

Stage A - service-like screen

1. Equilibrate at 25 C for 15 minutes.
2. Heat to 65 C at approximately 0.5 C/min.
3. Hold at 65 C for 30 minutes.
4. Cool to 25 C at approximately 0.5 C/min.
5. Hold at 25 C for 15 minutes.
6. Repeat for 10 cycles per cell.

Stage B - over-temperature robustness

Repeat Stage A with an 80 C maximum. Survivors complete 10 cycles per cell. This reproduces the harsher maximum used in the 2024 nucleator study and exposes hydrate deactivation that a 65 C screen may miss.

Stage C - route qualification

The best surviving condition from each route completes 50 additional cycles at the selected service profile. Any progressive decline is reported by cycle number and is not averaged away.

Measurements

For every cycle record:

- actual heating and cooling rate;
- maximum temperature and dwell;
- melting onset and plateau midpoint;
- minimum temperature immediately before crystallization;
- crystallization onset, peak, and induction delay;
- supercooling;
- temperature-time integral or another fixed relative heat-release proxy;
- trigger type, time, duration, and local temperature where applicable;
- specimen mass before and after each ten-cycle block;
- visible phase separation, residue, bubbles, corrosion, leakage, or colour change;
- sensor or fixture faults.

Calculate supercooling as:

melting plateau midpoint - minimum temperature immediately before crystallization exotherm

The relative heat-release proxy must use the same cell geometry, specimen mass, probe placement, cooling profile, baseline algorithm, and integration limits for every comparison. It is not a substitute for DSC enthalpy.

Data schema

Use one CSV row per cycle with these stable fields:

```
specimen_id,batch_id,route,composition,cell_id,cycle,
max_temp_c, dwell_min,heat_rate_c_min,cool_rate_c_min,
melt_mid_c,nucleation_c,supercooling_c,induction_s,peak_c,
release_proxy,trigger_type,trigger_time_s,trigger_local_c,
mass_before_g,mass_after_g,separation,leakage,corrosion,
visual_notes,fixture_fault,pass
```

Store raw time-series data separately with timestamp, specimen temperature, bath temperature, ambient temperature, heater command, and trigger state.

Common acceptance gates

Automatic-recovery gate

A condition passes only when all criteria are met:

- 30 successful crystallizations from 30 initial cycles across three cells;
- median supercooling no greater than 5 C;
- no individual cycle above 8 C supercooling;
- relative heat-release proxy at least 90% of SAT-SEED+;
- mass change no greater than 0.2% per ten-cycle block;
- no persistent phase separation, leakage, gas generation, or progressive drift;
- no dependence on undocumented agitation or operator handling.

On-demand gate

A triggered condition passes only when all criteria are met:

- remains liquid throughout a 60-minute pre-trigger hold at 25 C;
- crystallizes within 60 seconds of the trigger in at least 29 of 30 trials;
- relative heat-release proxy at least 90% of SAT-SEED+;
- no accidental trigger during the defined handling sequence;
- remains effective after both 65 C and 80 C stages;
- no leakage, corrosion, persistent separation, or progressive drift.

Failure of a gate does not make the material useless. It prevents that route from being credited for the stated Rumi behavior.

Route 1 - chemical nucleators

Initial screen

Each formulation totals 5.000 g. Percentages are mass fractions of the complete specimen, not additive mass relative to a separate 5 g SAT charge.

Specimen ID	SAT mass	Candidate mass	Candidate fraction	Basis
SAT-SS5	4.750 g	0.250 g anhydrous sodium sulfate	5.0 wt%	2026 SAT-SS literature starting point
SAT-CA05	4.975 g	0.025 g calcium chloride dihydrate	0.5 wt%	2024 reliable low-loading result

Specimen ID	SAT mass	Candidate mass	Candidate fraction	Basis
SAT-MG5	4.750 g	0.250 g magnesium chloride hexahydrate	5.0 wt%	2024 screen comparator
SAT-PP1	4.950 g	0.050 g tetrasodium pyrophosphate decahydrate	1.0 wt%	Prior SAT screening literature
SAT-BX1	4.950 g	0.050 g borax decahydrate	1.0 wt%	Prior SAT screening literature
SAT-NC4	4.800 g	0.200 g additive-free sodium chloride	4.0 wt%	2021 household-accessible result

Thoroughly combine dry solids without intentionally grinding hydrate crystals into an uncontrolled particle distribution. Seal, label, photograph, and weigh each prepared cell. If preparation requires melt blending, use the same mixing temperature, time, and agitation for every replicate and document the procedure before the series begins.

Candidate interpretation

- SAT-SS5 is the accessible Plan-B lead. Evidence reports supercooling near 4.1 C at 5 wt%, but the work is new and must be reproduced locally.
- SAT-CA05 is the strongest current comparator. The 2024 study found reliable nucleation through repeated 80 C cycles at 0.5 wt%.
- SAT-MG5 is expected to expose a failure mode: the 2024 study found initial operation followed by deactivation during 80 C cycling.
- SAT-PP1 and SAT-BX1 retain alternatives from prior literature but are not assumed equivalent to DHPD.
- SAT-NC4 tests the strongest ordinary household candidate using additive-free salt.

Optimization

Advance at most the best two candidates. For each passing starting formulation:

1. retain the passing concentration;
2. test one half-concentration condition;
3. test the midpoint between those concentrations;
4. select the lowest concentration that still passes the complete gate.

Do not optimize a failed candidate by combining it with another nucleator. Binary systems become a separate later route with new formulation IDs.

CMC integration

After a nucleator passes alone, prepare a 5.000 g specimen containing:

- the successful nucleator at its selected total-mass fraction;
- 0.025 g CMC-Na, equal to 0.5 wt%;
- SAT as the balance.

Repeat Stages A, B, and the automatic-recovery gate. Record CMC viscosity grade, degree of substitution if supplied, moisture, purity, lot, SDS, and certificate-of-analysis status. Do not use cross-linked croscarmellose sodium as CMC-Na.

Household candidate annex

Household availability does not waive identity control. These candidates are screening leads, not kitchen recipes.

Candidate	Possible source	Required identity check	Decision
Sodium chloride	Pickling/canning salt	Ingredient list states sodium chloride without iodine or anticaking additives	Include as SAT-NC4
Calcium chloride dihydrate	Pickling firmer, pool product, deicer	Product or SDS specifically identifies $\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$; mixed hydrates are not equivalent	Include only when exact hydrate is confirmed
Borax decahydrate	Laundry booster	Pure sodium tetraborate decahydrate; no fragrance or detergent blend	Include as SAT-BX1 when verified
Magnesium chloride hexahydrate	Nigari or bath flakes	Exact hexahydrate, additives listed, lot traceable	Comparator only
Potassium sulfate	Garden fertilizer	High-purity K_2SO_4 with contaminant analysis	Literature lead; defer from initial matrix
Activated alumina	Desiccant media	Gamma phase, particle size, purity, and absence of indicator dye	Literature lead; defer from initial matrix

Baking soda, washing soda, chalk, Epsom salt, detergent mixtures, charcoal, and graphite are excluded from the initial household screen because identity, evidence, or attribution is inadequate for this protocol.

Route 2 - retained SAT seed

Principle

A true SAT seed must remain solid SAT trihydrate while the main charge fully melts. The route converts a sourcing problem into a thermal-isolation problem.

Two-zone proof cell

Build a transparent, vertical development cell with:

- lower chamber containing 5.000 g pure SAT;
- upper seed pocket containing 0.050-0.100 g verified SAT trihydrate from a recorded batch;
- narrow communication neck permitting crystal propagation but discouraging bulk convection;
- external copper heat sink attached only to the seed pocket;
- independent main-charge and seed-pocket temperature probes;
- an otherwise identical ROUTE-BLANK cell with an empty pocket.

The proof cell is a laboratory fixture, not the cartridge design.

Thermal-isolation gate

Run the cell empty of SAT first. The main-charge location must reach and dwell at 65 C, then 80 C, while the seed-pocket location remains below 55 C. Reject the geometry when:

- the seed-pocket margin above 55 C is less than 3 C at any steady condition;
- the temperature difference depends on manual cooling;
- condensation, convection, or leakage can carry seed into the main chamber;
- the neck blocks or traps pressure.

After an empty-fixture pass, add SAT and verify visually that the retained seed remains solid through a complete main-charge melt. Then apply Stages A and B plus the automatic-recovery gate.

Inspect after every ten cycles for seed consumption, dehydration, neck blockage, trapped bubbles, and permanent cold-spot penalties. Advance only if no seed replenishment is required.

Route 3 - on-demand triggering

Shared pre-trigger condition

Use pure SAT without a chemical nucleator. Fully melt the charge, cool it to 25 C, and hold for 60 minutes. Any spontaneous crystallization before the commanded event is an accidental trigger and a failed trial.

Localized cold spot

- Apply a repeatable external copper cold finger to one marked cell location.
- Maintain the cold finger at 0-5 C.
- Log local wall temperature, bulk temperature, application time, onset delay, and full response.
- Apply for 60 seconds. If no response occurs, repeat in 60-second increments to a maximum total of five minutes.
- Use fixed contact pressure and interface material for all trials.

Reject the concept if it requires bulk temperatures, cooling energy, or trigger duration unsuitable for a future cartridge, or if ice/condensation makes the result non-repeatable.

Mechanical snap disk

- Use intact disks recovered from documented commercial reusable SAT hand warmers.
- Record source product, disk dimensions, material description if known, and prior service history.
- Use a cell geometry that permits one repeatable flex event without opening the cell.
- Flex once after the 60-minute hold and log onset.
- Inspect every ten cycles for corrosion, fatigue, abrasion, accidental triggering, and interference with sensing.

Do not fabricate an improvised disk until the commercial mechanism establishes a control response. A passing active trigger remains a fallback or commanded-release capability; it does not replace automatic recovery without a later thermal-policy decision by Tristan.

Down-selection

Rank passing routes using:

Criterion	Priority
Complete crystallization reliability	Critical
Supercooling and cycle-to-cycle spread	Critical

Criterion	Priority
Heat-release proxy and drift	Critical
Hydration and mass retention	Critical
Containment and corrosion burden	Critical
Material availability and identity	High
Passive operation and cartridge simplicity	High
Trigger controllability	Secondary unless commanded release is selected

Selection order:

1. Prefer a passing chemical nucleator for automatic recovery because it needs no moving part or isolated seed geometry.
2. Retain the retained-seed route when it matches reliability without consumables and remains manufacturable.
3. Retain cold-spot or snap-disk triggering as recovery or controlled-release research.
4. Preserve pure SAT and beeswax as controls throughout cartridge development.

Only after nucleation plus CMC passes may thermal-conductivity work begin:

- characterize commercial expanded graphite first;
- characterize BDG-01 independently using its specimen record;
- add only one heat-transfer variable at a time;
- calculate natural-ore formulations using total processed BDG-01 mass, not estimated graphite content;
- repeat crystallization, separation, corrosion, and mass-retention testing.

No route receives Rumi duty-cycle credit until cartridge-scale dummy testing covers containment, orientation, passive and fan-assisted recovery, blocked airflow, sensor faults, corrosion, and extended cycling.

Safety and stop conditions

- Wear eye protection and suitable gloves for hot vessels and hydrated salts.
- Use secondary containment and a stable guarded bath/heater.
- Keep chloride-bearing candidates isolated from ACE, pulse hardware, and unprotected metals.
- Stop on leakage, unexpected pressure, gas generation, sharp odour, glass damage, uncontrolled boiling, sensor disagreement, or over-temperature cutoff activation.
- Do not open a hot cell or force a stuck closure.
- Do not dry, crush, or substitute a hydrate without updating its material identity.
- Keep BDG-01 dust out of this programme until its separate wet, dust-controlled characterization is complete; possible sulfides, silica, and tremolite are relevant hazards.
- No experiment may depend on firmware as its only over-temperature protection.

References and evidence status

1. J. Li, M. A. Parkes, and C. G. Salzmann, "Extensive Screening and Performance Testing of Nucleating Agents for the Sodium Acetate Trihydrate Phase-Change Material," *Crystal Growth & Design* 24 (2024), 8292-8300. DOI: [10.1021/acs.cgd.4c00691](https://doi.org/10.1021/acs.cgd.4c00691). Local open manuscript: Chemistry/References/Li_2024_SAT_Nucleating_Agents.pdf.
2. W. Hua et al., "Preparation and Performance Analysis of Modified Sodium Acetate Trihydrate," *Materials* 11 (2018), 1016. Local open copy: Chemistry/References/2018_Modified_SAT_Nucleators_Thicke
3. H. Zhang et al., "Sodium acetate trihydrate phase change material with low undercooling," *Journal of Energy Storage* (2026), article 123777. DOI: [10.1016/j.est.2026.123777](https://doi.org/10.1016/j.est.2026.123777). Evidence used

- here: 5 wt% anhydrous sodium sulfate screening formulation and reported 4.1 C supercooling.
4. Z. Zhang et al., "Sodium acetate trihydrate-based composite phase change material with enhanced thermal performance for energy storage," *Journal of Energy Storage* 34 (2021), 102186. DOI: [10.1016/j.est.2020.102186](https://doi.org/10.1016/j.est.2020.102186). Evidence used here: 4 wt% NaCl and 3 wt% CMC literature formulation; this protocol tests NaCl before CMC.
 5. NanoArc, Chemistry/Proposals/NanoArc_RevB_RevC_PCM_Development_Proposal.pdf, draft dated 2026-08-11.
 6. NanoArc, Chemistry/Proposals/NanoArc_PCM_Cartridge_PCM_Reconciliation.md, dated 2026-08-12.
 7. Alphachem, Chemistry/SDS/Sodium_acetate_trihydrate.pdf and Chemistry/SDS/Anhydrous_sodium_sulfate.pdf
- Reference and SDS retrieval gaps are recorded in ../References/REFERENCE_GAPS.md and ../SDS/SDS_GAPS.md.

Evidence labels

- **Literature-backed starting point:** composition or behavior was reported by a cited study but remains unverified in NanoArc apparatus.
- **NanoArc experimental proposal:** geometry, gate, or method defined here for controlled testing; not a published result.
- **Approved formulation:** none at Rev0.
- **Implemented cartridge:** none at Rev0.

Approval and completion record

This protocol becomes active only after Tristan approves the fixture, materials, safety controls, and first test matrix. Completion of a route requires raw data, specimen records, photographs, failure notes, and a signed down-selection decision. A shared document entry or a successful isolated cycle is not implementation evidence.