Lab Handout -HEA Acoustic Signature → Interface & FGM Screening

Purpose (what you get): a fast, reproducible pre-screen that converts temperature-resolved 1D fingerprints into:

- **Level-1 labels** per interface (A/B): `co-evolution-compatible`, `interface-risk`, `dead-stable`, `breathing-switcher`, `high-noise-sensitive`
- **Level-2 actions**: what to test next (buffer layer, thermal cycling, process-window scan, repeatability checks)
- Optional: **FGM chain** suggestion + **buffer layer Top-K**

What it is not: not a replacement for CALPHAD/DFT/MD; not a mechanism proof; it is a conservative decision filter.

Lowest bar to try (what we need from a lab):

- 1 anchor alloy + 3–8 candidate alloys
- temperature-series 1D fingerprints on a consistent axis/grid (XRD/PDF/transport vs T all work)
- we run a first screening and return an edge matrix + buffer suggestions (typically 1–3 working days for a small set)

A. Minimal measurement set (lowest-friction adoption)

A1) One anchor alloy (baseline)

Pick an “anchor” alloy in your family (e.g., your baseline HEA composition). Measure a temperature series:

- $\{f_T(x)\}_T$ on a **common axis** (e.g., XRD 2θ grid)
- Suggested N_T: 10–30 temperatures over the relevant window

A2) Candidate alloys (screen set)

For each candidate composition, measure a matching temperature series on the **same axis/grid**.

If you only have room for a very small set:

- 8–12 temperatures is enough to start (but window-gating and breathing get better with more points).

A3) Optional: interface pairs you care about

If screening for multilayers/joins/FGM, define endpoint pairs (A,B) up front.

B. How to run (in this folder)

B1) Generate the anchor signature (bands)

Use the notebook (recommended for external sharing):

- LabReady_HEA_Signature_Scoring_Workbook.ipynb
- Run Section **13.3** then **13.3D**

Outputs:

- hea_acoustic_signature.json

B2) Transfer as a "filter" (single candidate vs anchor)

In the same notebook, run Section **13.4**.

Outputs:

- hea_signature_filter_transfer_demo.json

B3) Candidate pool → edge matrix → buffers → chain search

In the same notebook, run Section **13.5**.

Outputs:

- hea_fgm_edge_matrix_demo.json
- hea_fgm_edge_matrix_demo.csv

C. Metrics you'll see (what they mean)

Given two materials A and B:

Important: scores are computed in both directions (A→B and B→A). For interface decisions we take the worse side (more conservative).

1. **Resonance overlap** (static similarity in band space)

- `overlap_auc` is a temperature-weighted average overlap in band space (higher is better), but can be fooled by static look-alikes.

2. **Conflict** (incompatible co-evolution in the same filter)

- `conflict_auc` is a temperature-weighted average divergence in band space (lower is better).
- A **windowed conflict peak** (max conflict within the gated window) is a strong warning sign.

3. **Breathing alignment** (dynamic compatibility)

- `breath_sync` measures whether A and B “breathe” together vs temperature (higher/positive is better).
- `activity_ratio` compares overall breathing activity to the anchor/reference (too low → “dead-stable”; too high → noise-sensitive / turbulent).

4. **Stability proxy** (conservative combined score)

Used for ranking and FGM chain selection; do not interpret as a guarantee.

Critical practice: apply **temperature-window gating** around the transition/service window to avoid static-similarity false positives.

D. Level-1 label → Level-2 lab action (copy/paste)

Level-1 enum	Typical trigger	What to do next
`co-evolution-compatible`	overlap high, conflict low, breath_sync > 0, activity reasonable	proceed to interface thermal cycling + microstructure checks; keep 1–2 buffer backups
`interface-risk`	conflict_auc high or conflict peak in a window	search buffer/graded layer; scan process window (HT path, ramp rate, hold); prioritize interface cycling
`dead-stable`	overlap high but activity low, breath_sync weak	stimulation tests (thermal cycles / power pulses); avoid as key FGM node until proven

| `breathing-switcher` | breath_sync strong, conflict low, activity near anchor | prioritize perturbation tests; if conflict stays low, use as chain node candidate |

| `high-noise-sensitive` | activity extremely high / turbulent breathing; low repeatability | repeatability checks; vary ramp rate; improve sample/measurement before deciding |

E. Practical acceptance rules (recommended)

Avoid hard global constants; use **candidate-pool percentiles**.

A simple conservative rule-of-thumb:

- Flag `interface-risk` if conflict is in the top quartile of all edges OR a clear conflict peak exists in the gated window.
- Only treat an edge as "good enough" if stability is in the top quartile AND conflict in the bottom quartile AND breath_sync > 0.

Wording note (to avoid overclaiming):

- We do not "predict phase transitions"; we **prioritize temperature windows** where mismatch or switching behavior is likely, then ask experiments to verify.

F. What to send (for a quick trial)

F1) If you only want to review the method (no data sharing)

Send (PDF/Markdown is fine) + the notebook:

- HEA-Acoustic-Signature_Lab-Handout_2pager.md
- HEA-Presence-to-Quantum-Breathing_Acoustic-Signature_Method-and-Findings.md
- LabReady_HEA_Signature_Scoring_Workbook.ipynb

F2) If you want us to run one screening pass (recommended)

Please provide either:

- **Option A (small pool):** 1 anchor alloy + 3–8 candidates (anonymized is fine), each as a temperature series $\{f_T(x)\}_T$ on a consistent x-grid.
- **Option B (targeted check):** 1 A/B interface pair you suspect is risky + 1 "known-stable" control pair.

Along with:

- the temperature list (K/°C) and measurement type (XRD/PDF/transport),
- the x-axis definition/units (e.g., 2θ) and whether curves are already background-corrected / normalized.

What you get back:

- a conservative interface summary (Level-1 labels + suggested next experiments),
- an edge-matrix CSV for scheduling, plus top buffer-layer suggestions when applicable.

F3) If you prefer to run it locally (self-run mode)

We can share the runnable notebook + expected inputs/outputs. To keep iterations fast and avoid “one-way drop-off”, please plan for one of:

- a 15-minute debrief call after the first run, or
- sending back the exported edge-matrix CSV + 2–3 sentences: “what matched / what didn’t / what data constraints we hit”.

If the pilot is useful, we’re happy to turn it into a short joint case study / methods note (or at minimum, agree on an acknowledgement / citation) so the effort is mutually beneficial.

Reciprocity (so this doesn’t become a “freebie PDF”): we’ll actively support the first run and iterate quickly; in return, please share outcomes (even anonymized) and align on acknowledgement/citation if this informs a decision, report, or publication.

Sharing note (practical): please don’t forward/redistribute the notebook outside your group without asking—happy to share broadly, but we want to track where it’s running so we can support and improve it.

G. Next step (if the lab wants to try)

Pick one real anchor + 3–8 candidates, then we run:

1. anchor signature (13.3/13.3D)
2. pool screening (13.5)
3. choose 1–2 “safe edges” + 1 “interface-risk” edge and validate via interface thermal cycling