# Towards a Physically Significant E45: Predictive Inclusion Assessment through FEM and Digital SEM


- RJ Lee, S. Story, M. Fuhrman, M. Potter, G. Casuccio, R Booth, A Capsambelis, S. Blanda, N. Parmar
- RJ Lee Group & United States Steel Corporation

“These results demonstrate directional, physically consistent relationships between inclusion characteristics and mechanical response; however, expanded datasets are required for predictive deployment.”

# Objectives

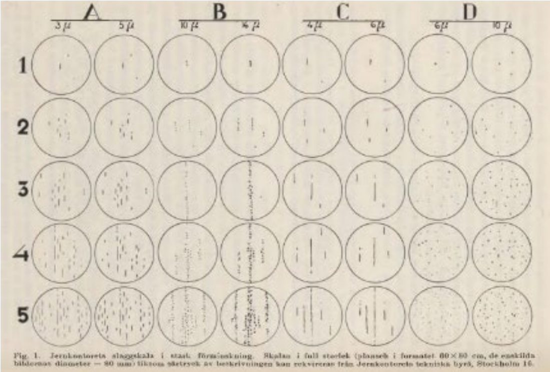
- Modernize inclusion rating methodology
- Correlate inclusion characteristics with mechanical performance
- Develop a predictive framework (E45') for steel quality assurance

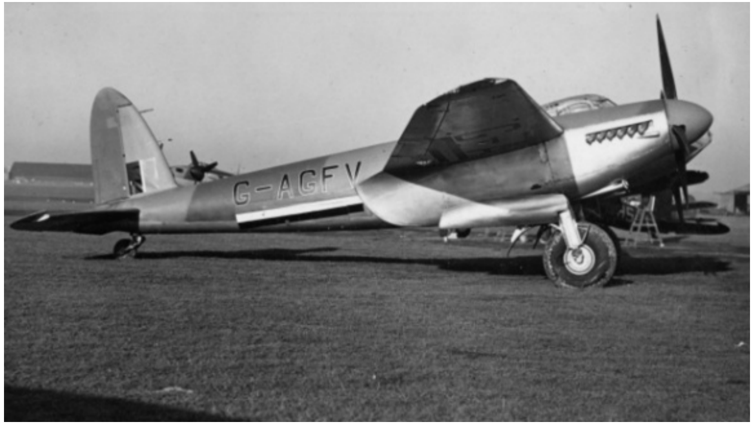
# Introduction

- Background on ASTM E45 and its role in steel inclusion rating
- Limitations of traditional visual rating methods
- Motivation for a predictive, performance-linked standard

# Background: JK Inclusion Ratings

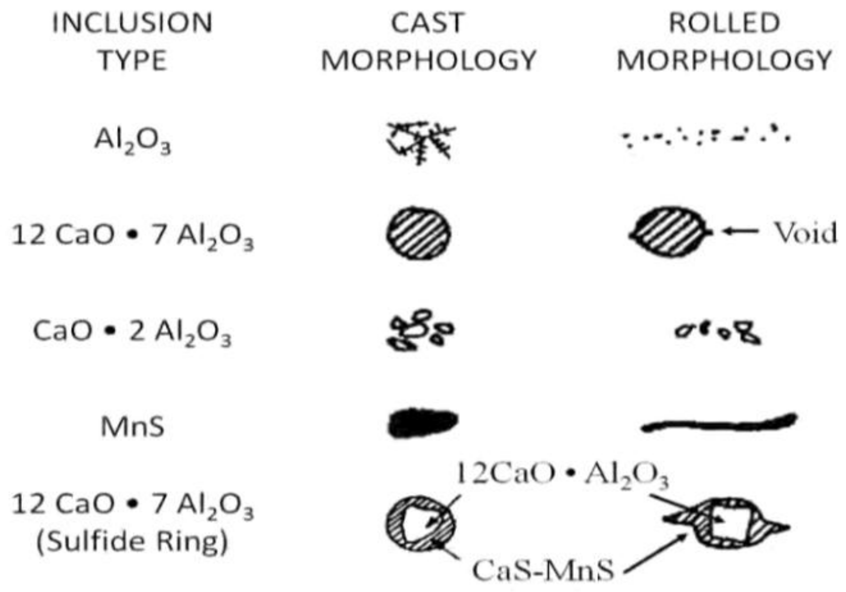
- Developed by Joel Larsson at Hofos (1927)
- The intended purpose was to evaluate quality of ball bearing grades
- Sweden supplied Germany with iron ore and precision ball bearings for WWII.
- Allies' nations needed to catch up to the German steel quality and to adopt their own interpretation of a steel cleanliness method: E45



# Background: E45 Rating Limitations

- Outdated Standard
  - Developed for forged ingots
- Descriptive, Not Predictive
  - Inclusion ratings based on visual inspection
  - Does not consider actual effect on mechanical properties
  - No consideration of microstructure
- Ignores Key Inclusion Characteristics
  - Size distribution
  - Spacing
  - Aspect ratio
  - Proximity to surface
- Limited Real-World Applicability

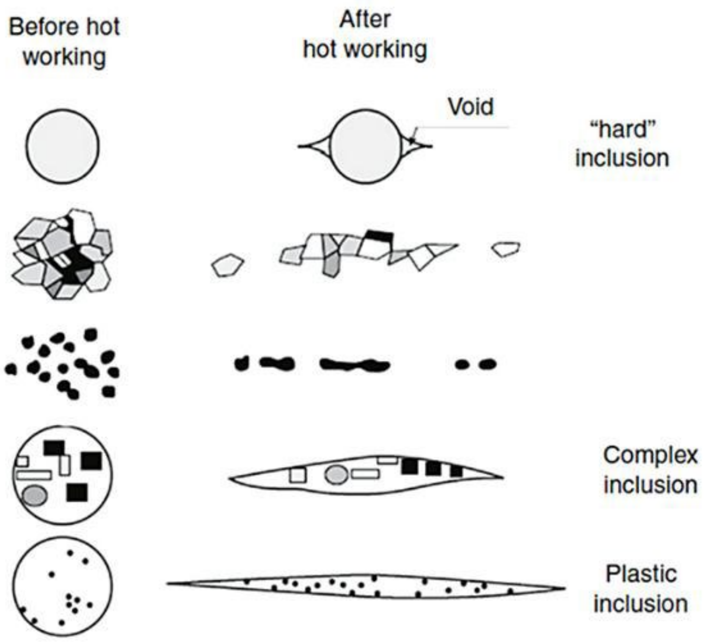



**Findley**

# Background: Motivation for “new” standard

- Does not reflect modern steel manufacturing methods
- Need a standard that accurately captures the total population of inclusions and can relate to their population to macro population

*Effect of Reduction*



# Materials & Methods

- E45 USS samples with corresponding optical E45 ratings
- ASCAT inclusion results with E2142 clustering
  - High-resolution imaging of inclusion morphology
  - Quantification of clustering and spatial distribution
- Finite Element Modeling (FEM)
- AI-Driven Data Integration via AKM-SEAMS®
  - Data fusion from FEM and SEM
  - Predictive analytics

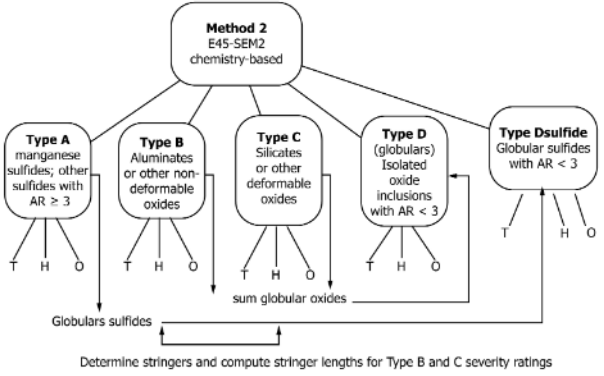
# Materials/Method: Heats/Samples Processed

- Four different heats of AHSS were selected
- Results from various tests include
  - Chemical analysis
  - Tensile
  - Hole Expansion
  - V Bending
  - Steel Cleanliness
    - Optical – ASTM E45
    - SEM – ASTM E2142
      - Inclusion analysis

# Materials/Method: Inclusion Analysis

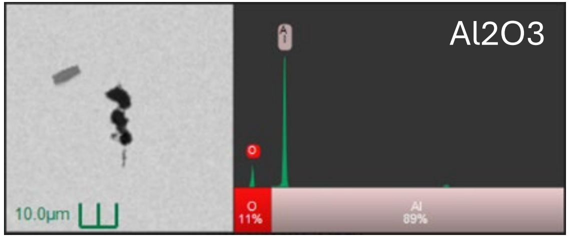
Inclusion analysis using field-emission SEM was performed with IntelliSEM and includes:

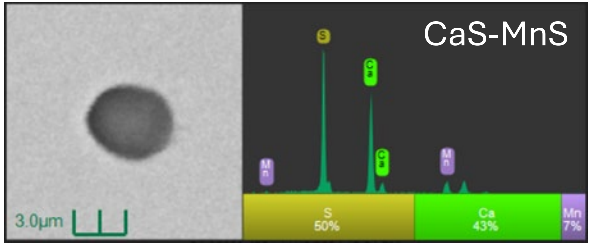
- High resolution images of individual inclusions
- Steel cleanliness characterization (E2142)
  - Worst field analysis
- Spatial distribution
- Clustering analyses

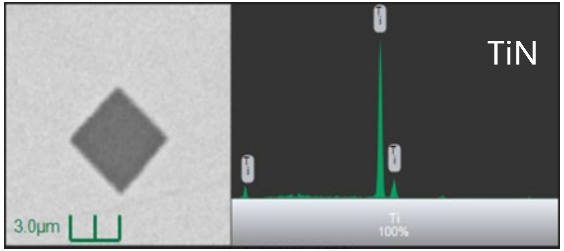


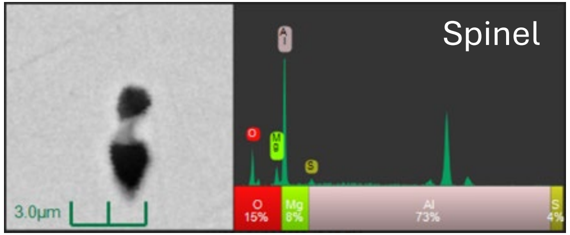

- Inclusion images were used for developing stress concentration factors (SCFs) with finite-element modeling (FEM)

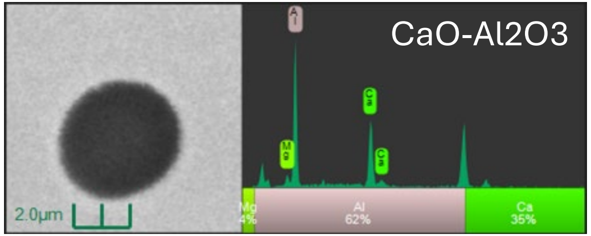
# Materials/Method: Inclusion Types

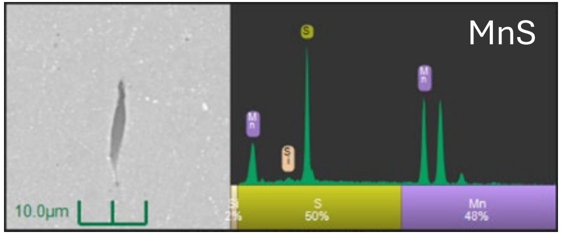


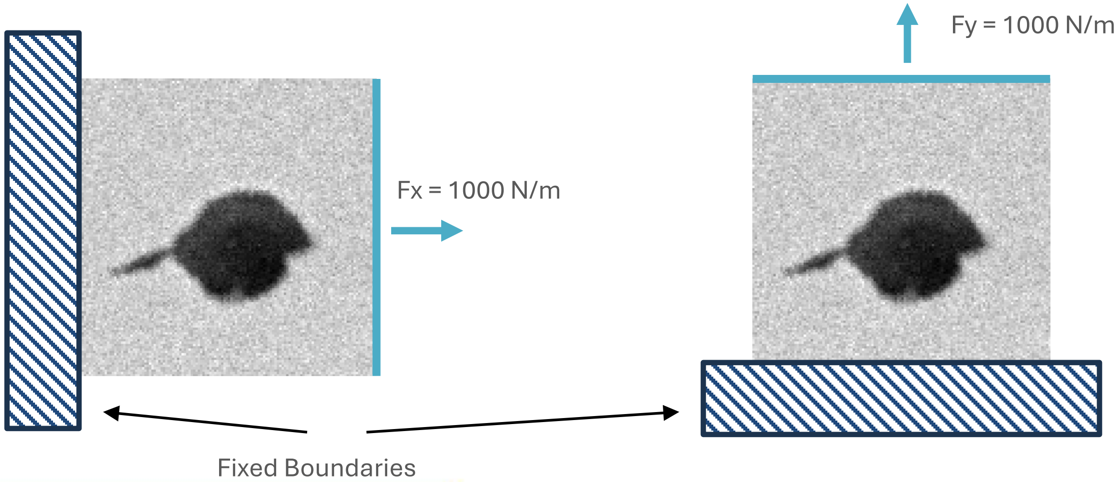



# Materials/Method: FEM with Elmer

- Elmer FEM is a very versatile, open-source, Multiphysics simulation tool.
- https://www.csc.fi/elmer
- Simulate linear elastic deformation under axial force of 2D surface containing void shaped as IntelliSEM inclusion




Elmer FEM

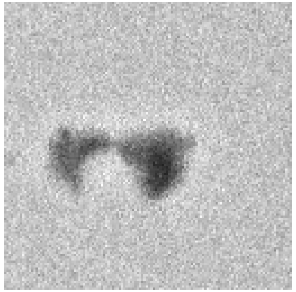
open source multiphysical simulation software

Young's Modulus = 193 Gpa

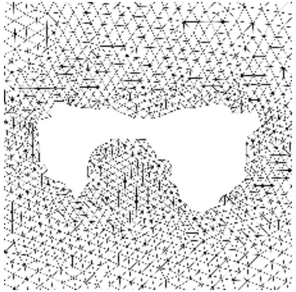
Poisson Ratio = 0.29

# Materials/Method: Workflow

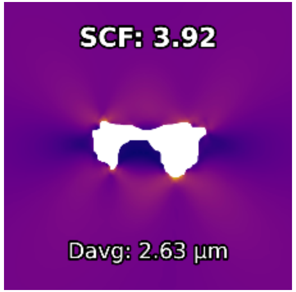
Raw Micro-Image



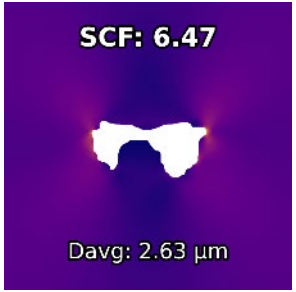
Mesh



x-axis Force

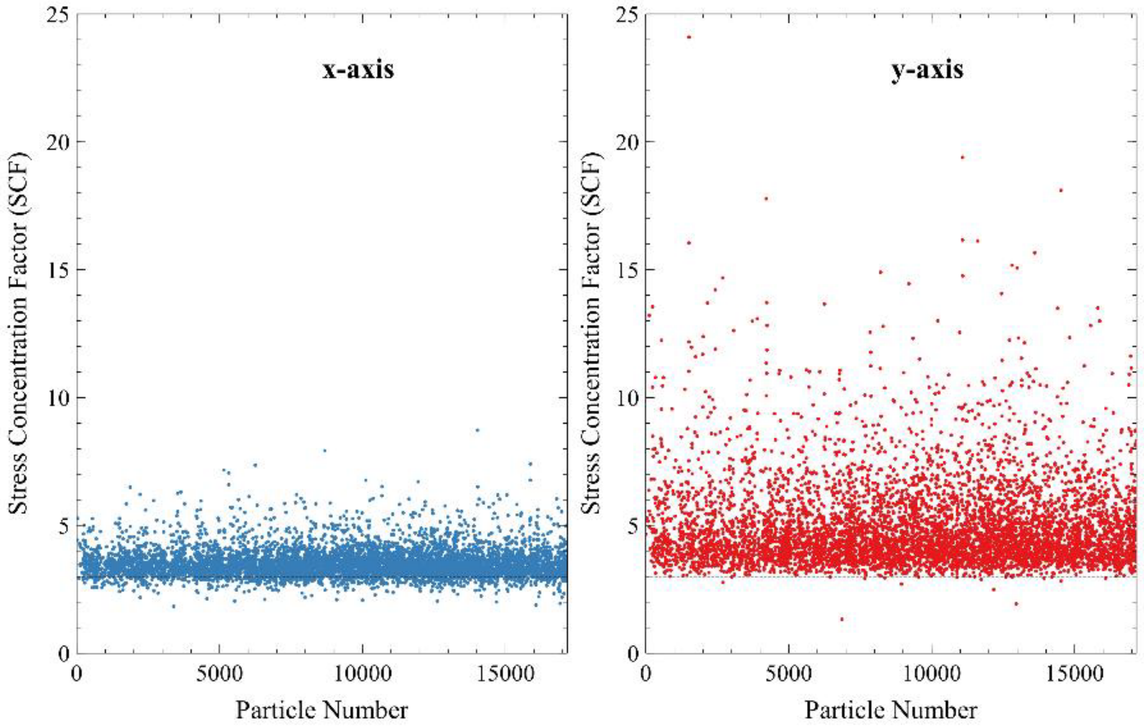



y-axis Force



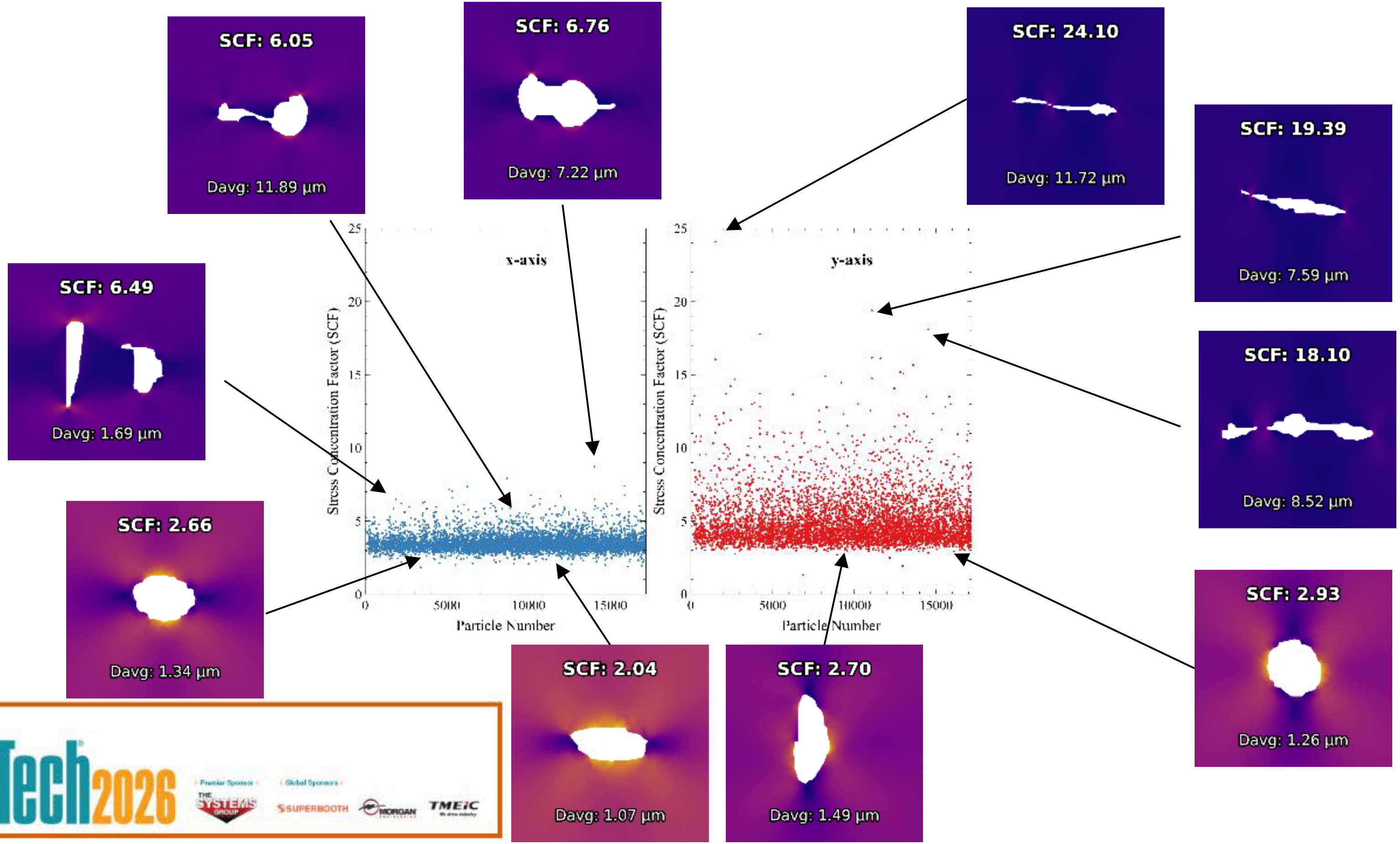

1. Export micro-images and tabular data.
2. Threshold, pad, and make binary image.
3. Extract contour and mesh region.
4. Apply boundary conditions and solve for Von Mises Stress with two, separate, axial forces.
5. Calculate stress concentration factor (SCF) by normalizing max Von Mises with void to Von Mises far from void.

# Materials/Method: Visualize SCF Distribution



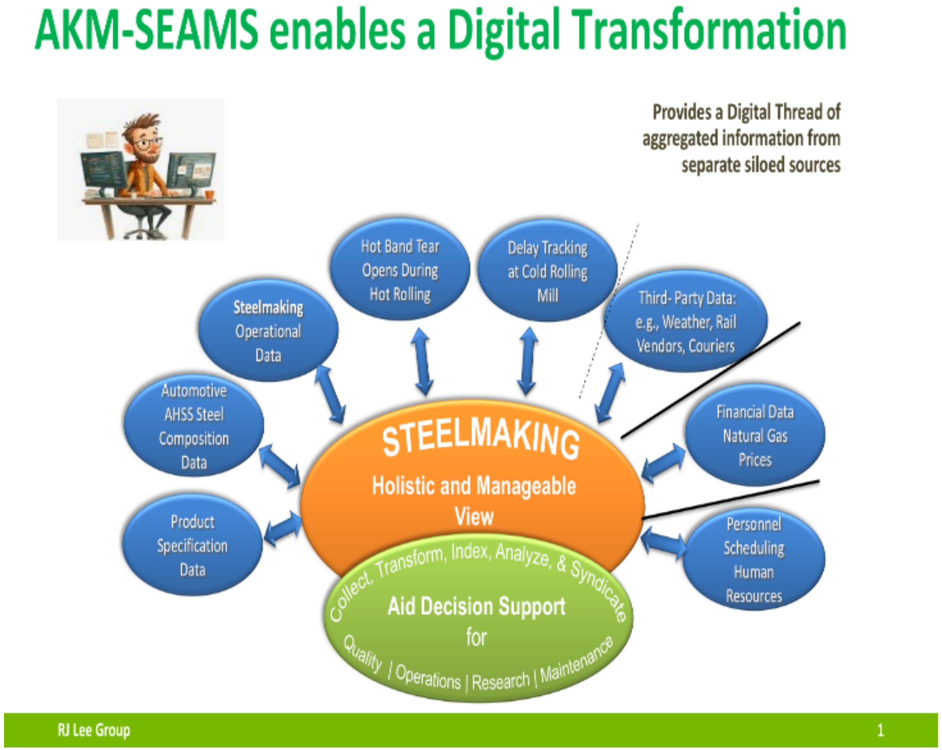

- Rolling direction is x-axis.
- Higher stresses perpendicular to rolling direction
- Outliers are high aspect ratio inclusions.

# Materials/Method: Visualize SCF Distribution



# AKM-SEAMS® – A Data Management Platform

- ***AKM-SEAMS*** - A Data Content and Augmented Knowledge Management platform that supports data ingestion from multiple disparate sources for ease of content discovery from one holistic view.
- ***AKM-SEAMS*** platform organizes and interlinks the data so you can easily find other, related data.
- Data analysis and analytics can be performed within ***AKM-SEAMS*** using machine learning algorithms and models to gain insights for authoritative decisioning.
- With the power of a built-in graph database, ***AKM-SEAMS*** enables exploring data relationships across and within Entities from multiple sources.
- ***AKM-SEAMS*** makes your data usable!



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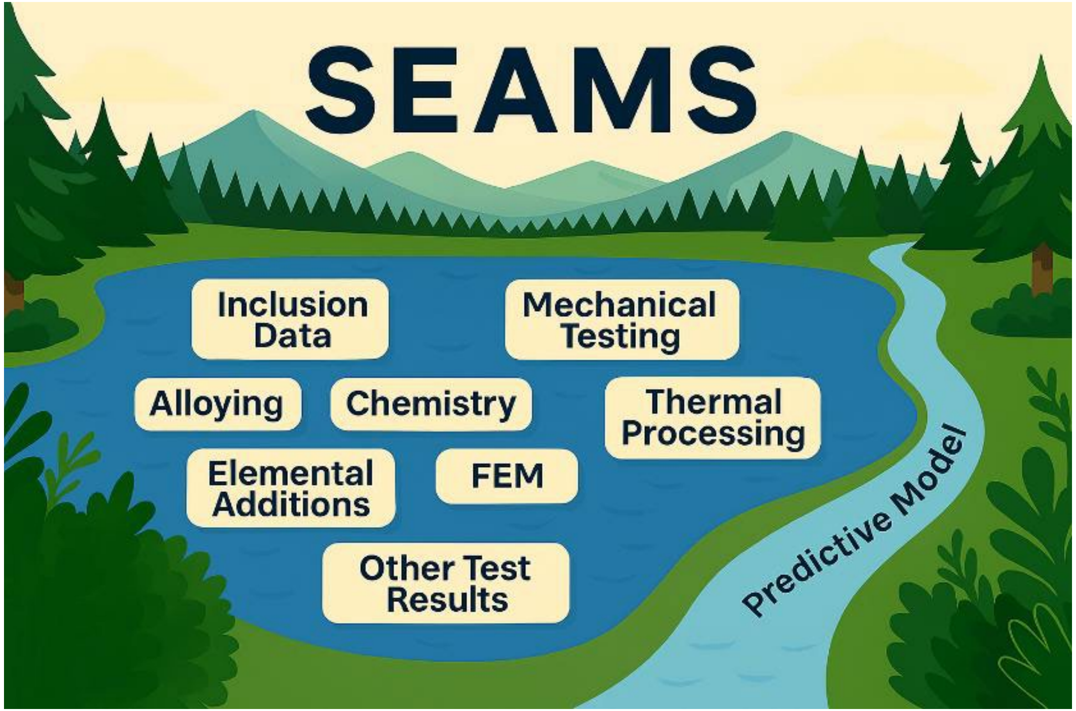
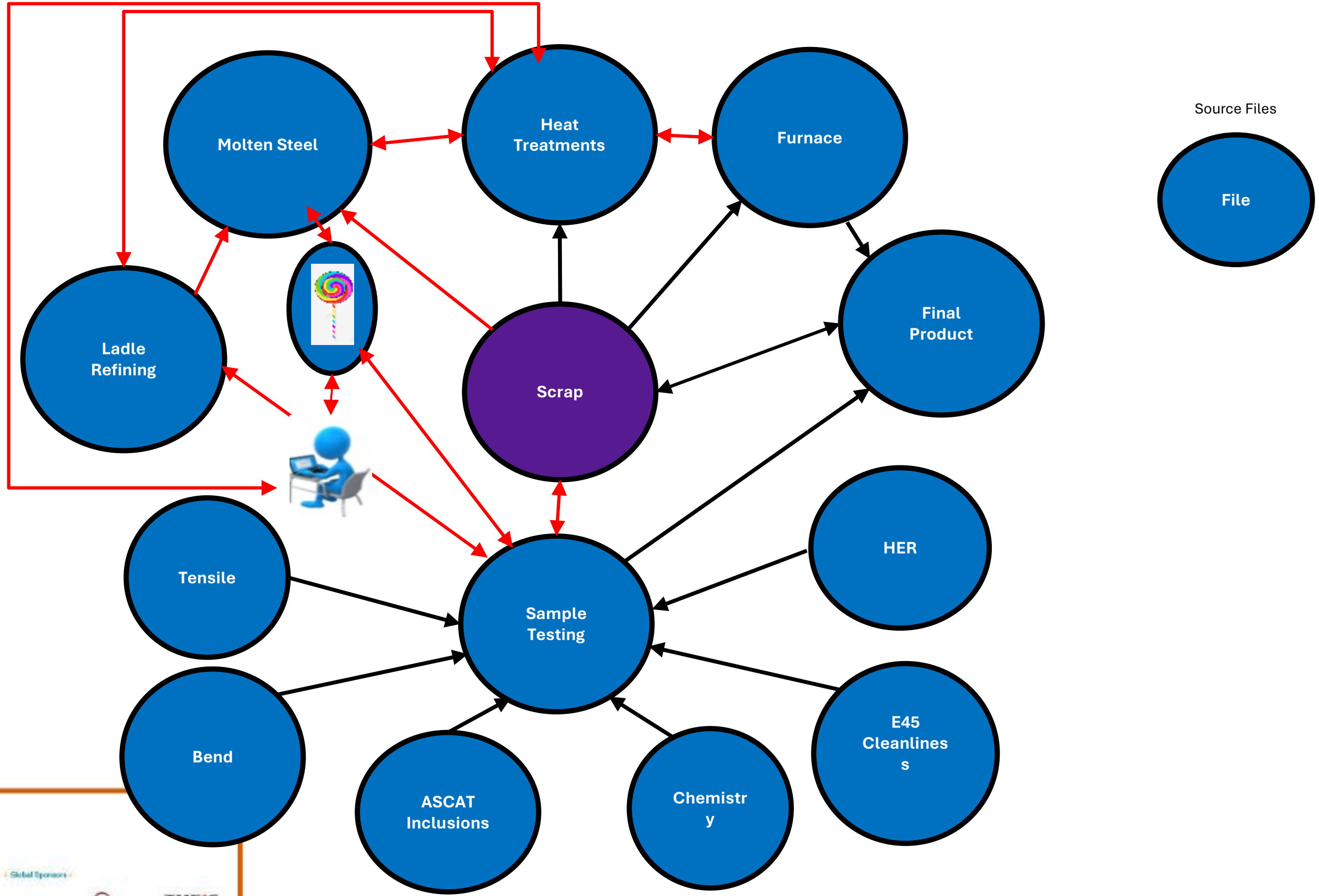
# Materials/Method: The Data Lake



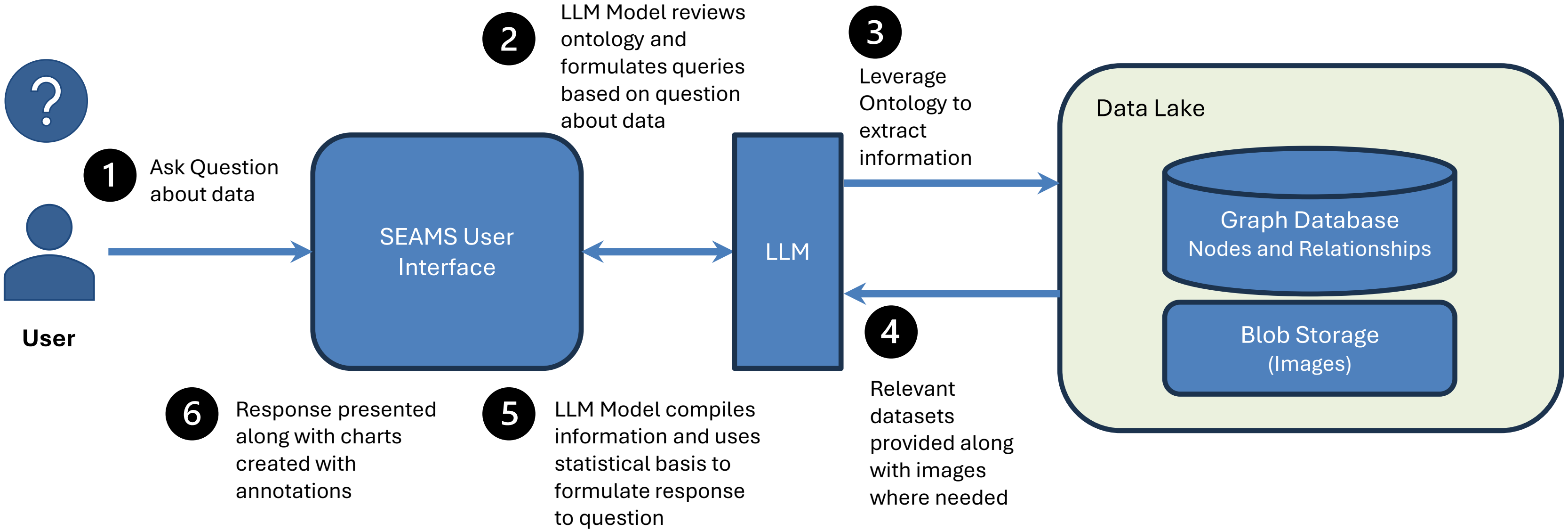
# Steel Ontology

**Data**

- Scrap Sources
- Electric Arc Furnaces
- Heat Treatments
- Molten Steel
- Ladle Refining
- Final Steel Products
- Samples
- Chemistry Tests
- E45 Cleanliness Tests
- E2142 Cleanliness Tests
- Inclusion Tests
- Hole Tests
- Bend Tests
- Tensile Tests



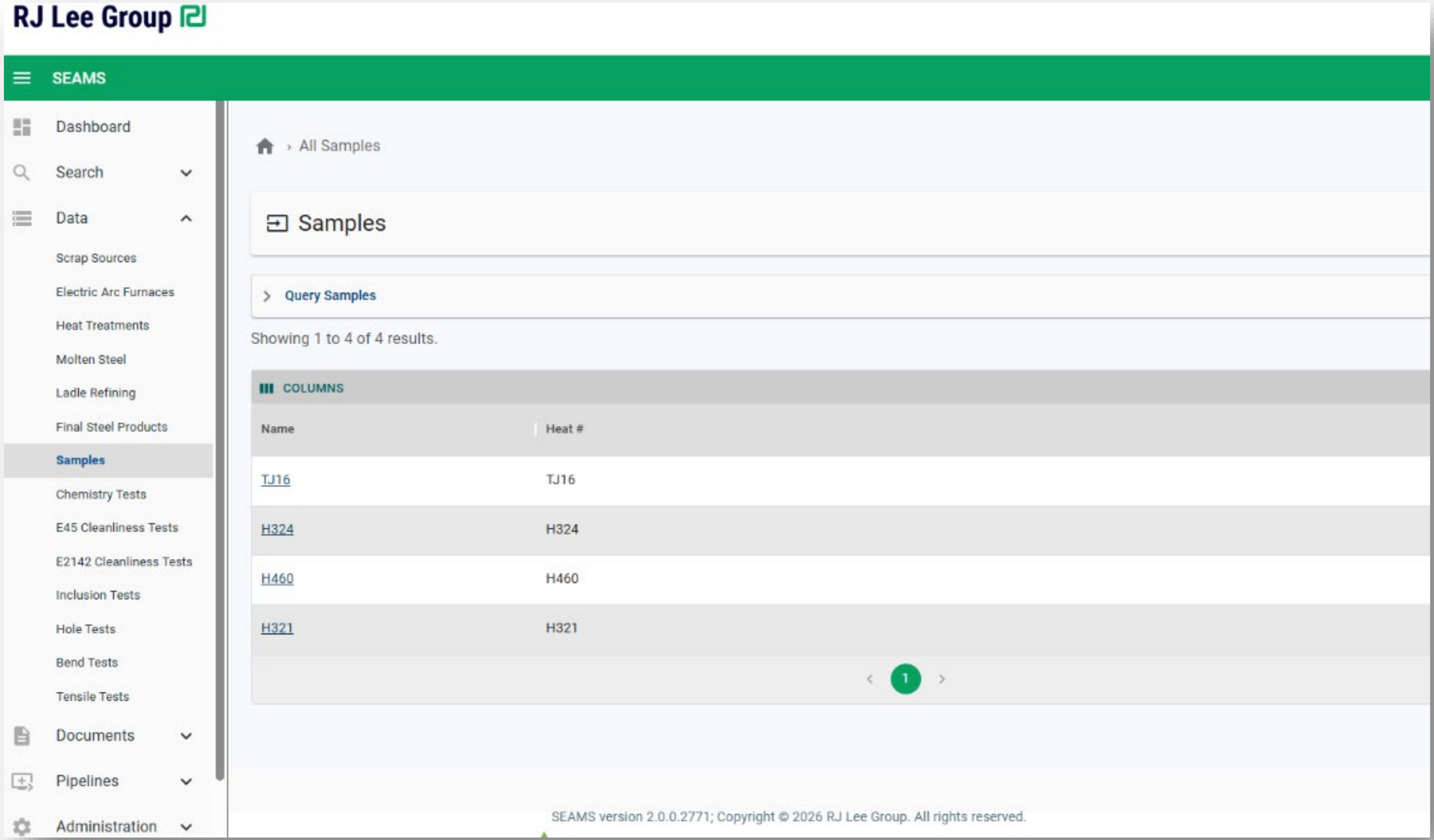
# Materials/Method: Querying the Data Lake



# Terms

- **Data Lake** – A centralized repository for storing structured and unstructured data at any scale for analytics
- **Graph Database** – A database that uses nodes and relationships to represent and query connected data *(e.g., heats, samples, test results)*
- **Blob Storage** – Cloud-based object storage for unstructured data such as SEM images and micrographs
- **Ontology** – A structured data model defining entities and relationships across the steel process (heats, samples, tests, products)
- **LLM** – Large Language Models are Natural Language Processing Artificial Intelligence Models
- **AKM – SEAMS** – The data lake platform with LLM that is used for the analysis
- **Stress Concentration Factor (SCF)** – Ratio of maximum Von Mises stress near an inclusion to the far-field stress, quantifying the mechanical severity of a defect
- **Calcium Modification Index (CaModIdx)** – Cation fraction Ca/(Ca+Al+Mg) for oxide-bearing inclusions; values near 1.0 indicate fully modified calcium aluminates
- **Inclusion Clustering** – Spatial grouping of non-metallic inclusions that can act collectively as a single larger defect under stress

# AKM-SEAMS: User Interface



# AKM-SEAMS: Question to LLM

Can we compare the mechanical properties with cleanliness ratings?

# Mechanical Features Comparisons

## Mechanical Feature Matrix

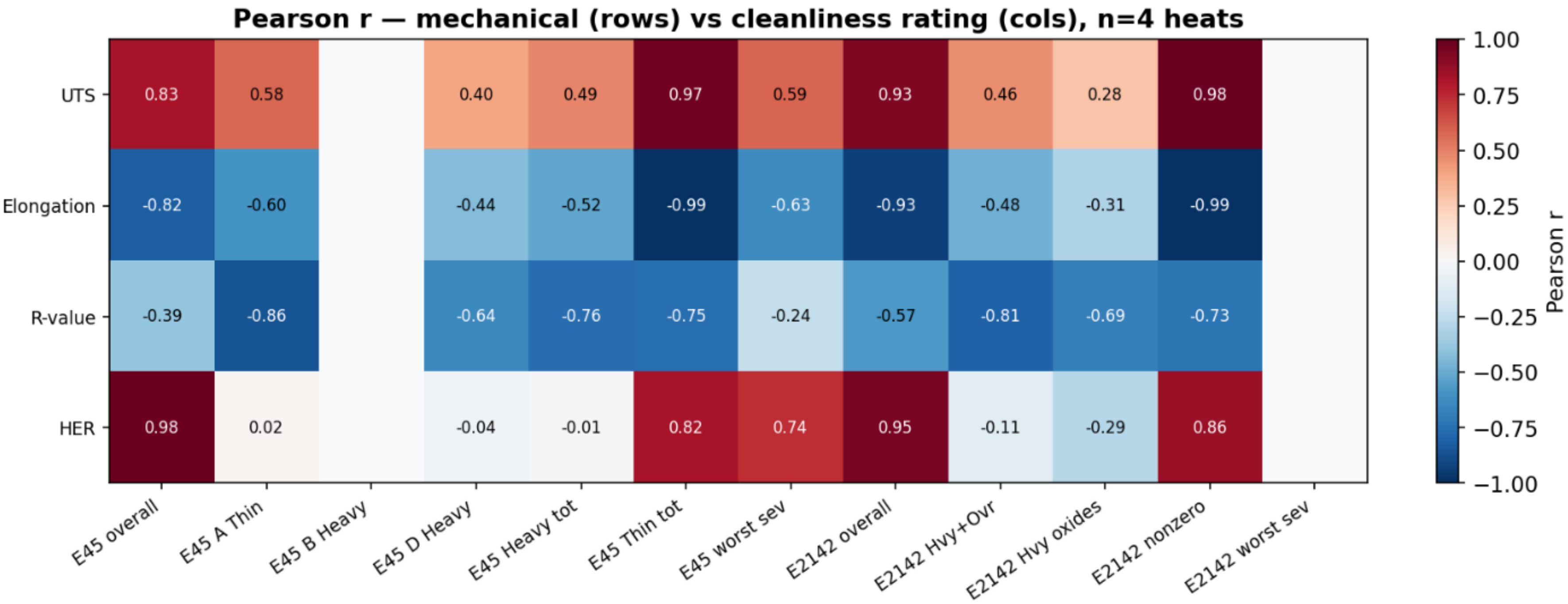
| Heat | UTS (MPa) | Elong (%) | R | HER |
|---|---|---|---|---|
| L-01 | 1018 | 9.7 | 0.84 | 0.24 |
| L-02 | 1009 | 10.4 | 0.80 | 0.17 |
| H-01 | 1585 | 3.1 | 0.70 | 0.26 |
| H-02 | 1584 | 3.4 | 0.77 | 0.36 |

# Per-heat summary - Mechanical means and cleanliness scalars

*UTS in MPa; HER as fraction; severity-sums = Σ(severity × count). Counts (H+O, H-Ox) are integers.*

| Heat | n_T | UTS | Elong% | R | HER | E45 idx | E45 A·T | E45 B·H | E45 D·H | E2142 idx | E2142 H+O | E2142 H-Ox |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| L-01 | 9 | 1018 | 9.71 | 0.838 | 0.237 | 180.5 | 0.0 | 0.0 | 2.5 | 3190.0 | 297 | 295 |
| L-02 | 9 | 1009 | 10.38 | 0.797 | 0.170 | 150.0 | 0.0 | 0.0 | 0.0 | 3095.5 | 308 | 301 |
| H-01 | 6 | 1585 | 3.09 | 0.704 | 0.257 | 223.0 | 15.0 | 0.0 | 7.0 | 3404.5 | 761 | 716 |
| H-02 | 6 | 1584 | 3.36 | 0.768 | 0.356 | 321.5 | 0.0 | 0.0 | 0.0 | 3573.0 | 233 | 126 |

# Correlation matrix - All mechanical × cleanliness pairs



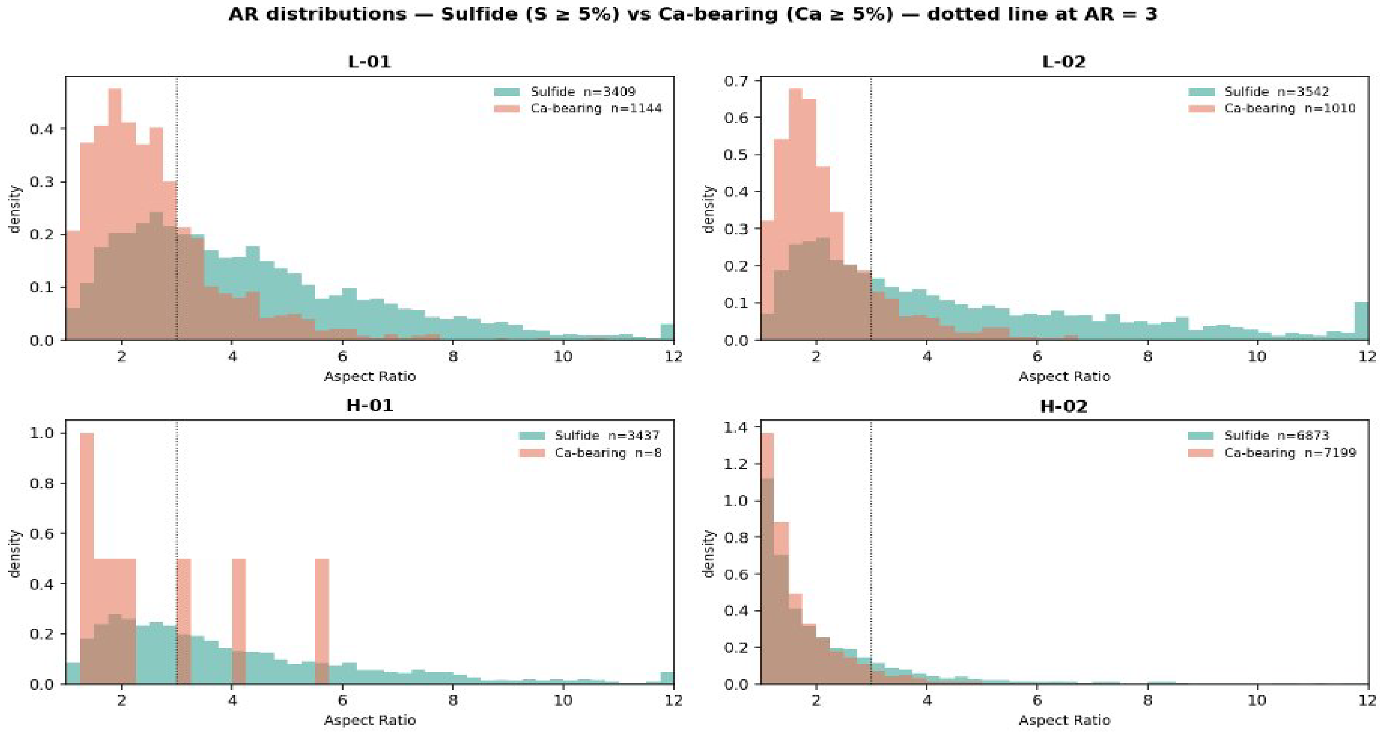

*Pearson r at heat level (n=4). Red = positive, blue = negative. Cells with |r| ≥ 0.9 are mostly driven by H-01/H-02 having the highest UTS but the lowest elongation; interpret with care.*

# AKM-SEAMS: Question to LLM

Can we compare the morphology of the Sulfides and Ca containing inclusions e.g. Max AR, Mean AR, %<3:1 , %>3:1?

# AR distributions per heat

Density histograms — dotted line = AR = 3 (stringer threshold).



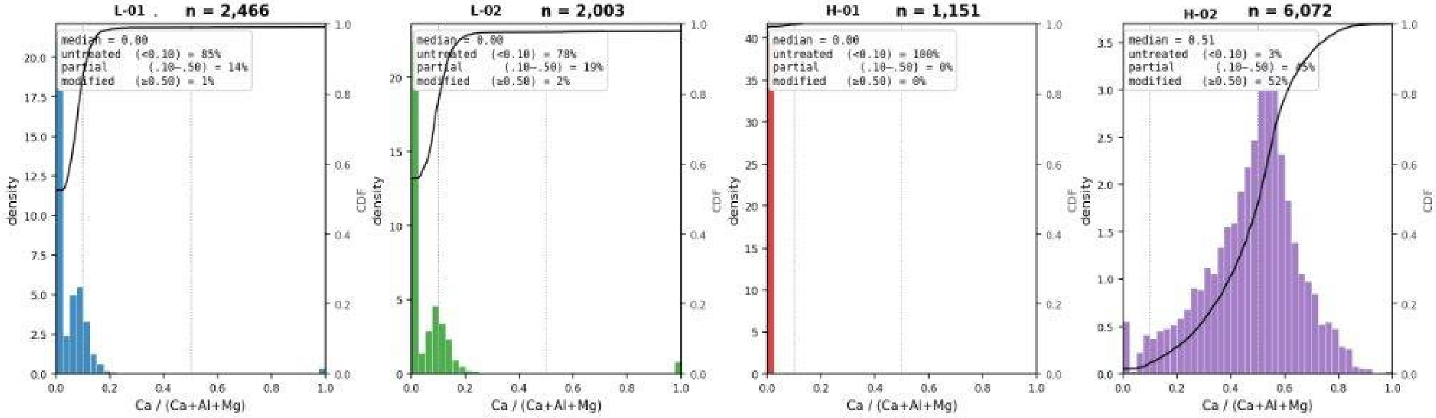

Ca-bearing curves (orange) sit tightly between AR 1–3 in every heat — calcium-modified inclusions are intrinsically equiaxed. Sulfide curves (green) show a long high-AR tail in L-01/L-02/H-01 and collapse onto the Ca-bearing curve in H-02, reflecting (Ca,Mn)S substitution in H-02's sulfides.

# AKM-SEAMS: Question to LLM

Can we quantify the effect of Ca addition?

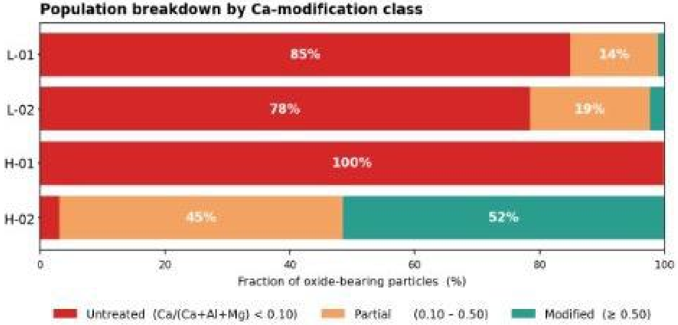
# Calcium Modification Index —- Oxide-Bearing Inclusions

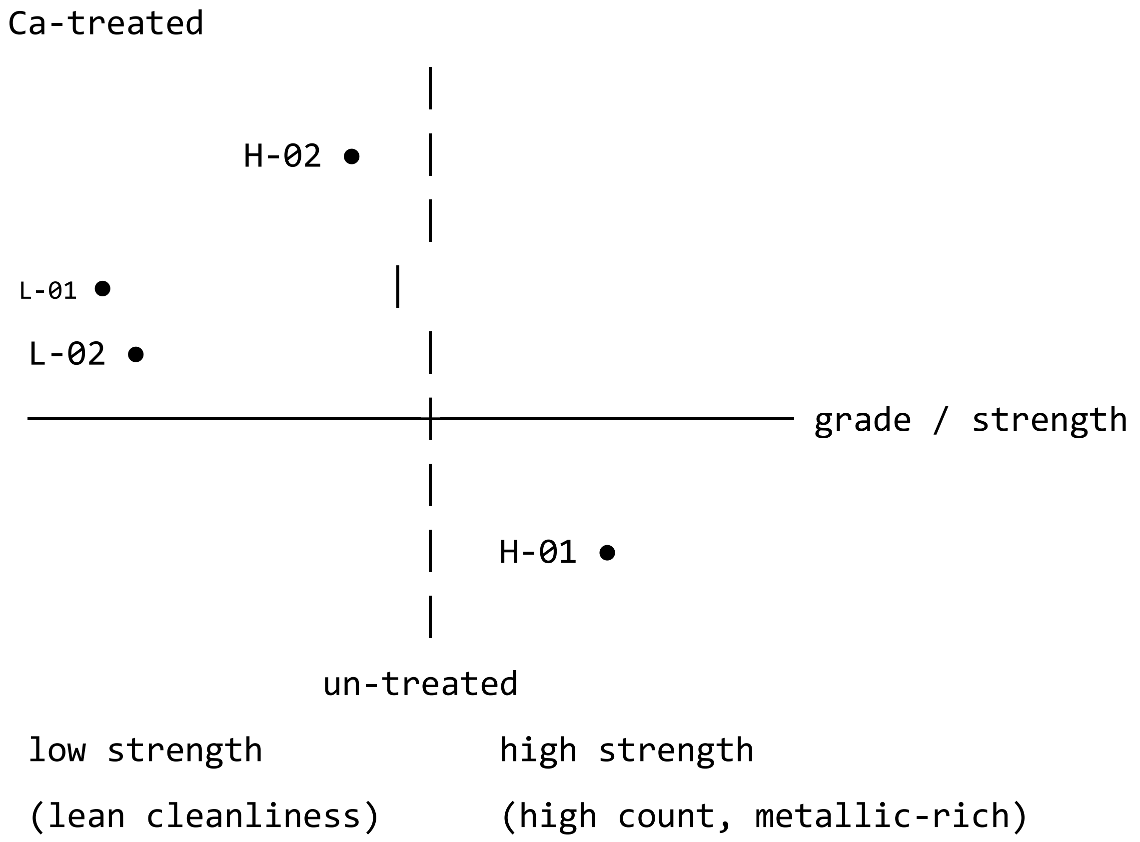
CaModIdx = Ca / (Ca + Al + Mg) cation-fraction per particle, computed for every inclusion with O ≥ 5 wt%.
A unimodal peak near 1.0 indicates fully Ca-modified calcium aluminates; a peak near 0.0 indicates surviving alumina.
Bimodality means partial modification — both populations co-exist in the heat.




Per-heat verdict

- L-01 : essentially un-treated — 1 % modified, 85 % untreated
- L-02 : essentially un-treated — 2 % modified, 78 % untreated
- H-01 : essentially un-treated — 0 % modified, 100 % untreated
- H-02 : partially Ca-modified — 52 % modified, 3 % untreated




Ca-treated
H-02
L-01
L-02
grade / strength
H-01
un-treated
low strength
(lean cleanliness)
high strength
(high count, metallic-rich)

# AKM-SEAMS: Question to LLM

What properties vary in the same manner in the two groups and is this variation physically sensible?

# AKM-SEAMS: Question to LLM

Does the inclusion composition correlate with mechanical properties?

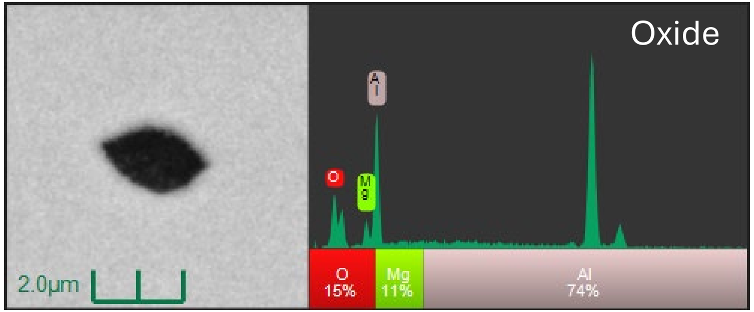
# Oxide classes - Definition by EDS thresholds

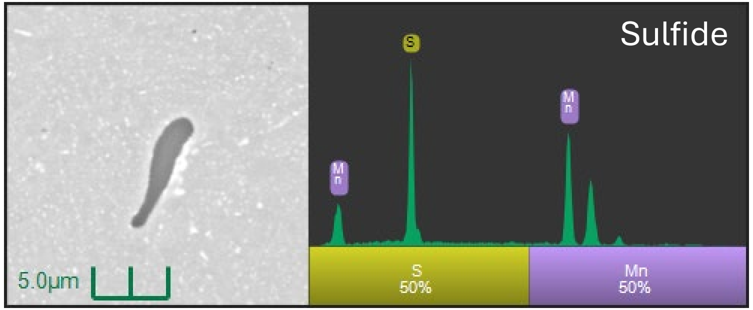
All cutoffs at 5 wt %, applied to the raw per-particle EDS readings.

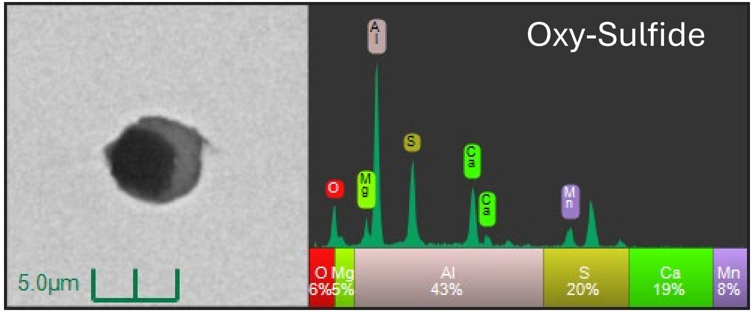
| Class | Rule | Meaning | Typical phases |
|---|---|---|---|
| **oxide** | O ≥ 5 % AND S < 5 % | Oxygen-bearing, no sulfur | $Al_2O_3$, $SiO_2$, calcium aluminates, $MgO{\cdot}Al_2O_3$ spinels |
| **oxysulfide** | O ≥ 5 % AND S ≥ 5 % | Both elements present | Typically a (Ca,Mn)S shell on an oxide core — **duplex inclusions** |
| **sulfide** | O < 5 % AND S ≥ 5 % | Sulfur-bearing, no oxygen | Pure MnS, (Ca,Mn)S |
| **metallic** | O < 5 % AND S < 5 % | Neither element above threshold | Fe-rich pickup, carbides, intermetallic phases |

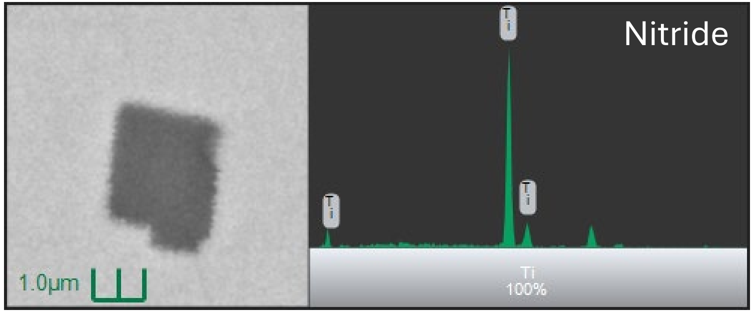
- Mutually exclusive — every particle lands in exactly one class; the four fractions sum to 100%.
- Same scheme is used in every project deck: 01_ca_modification_index, 02_inclusion_properties_by_type, 03_morphology_sulfide_vs_ca, and the within-pair variation analysis.

# Oxide/Sulfide: Inclusion Types



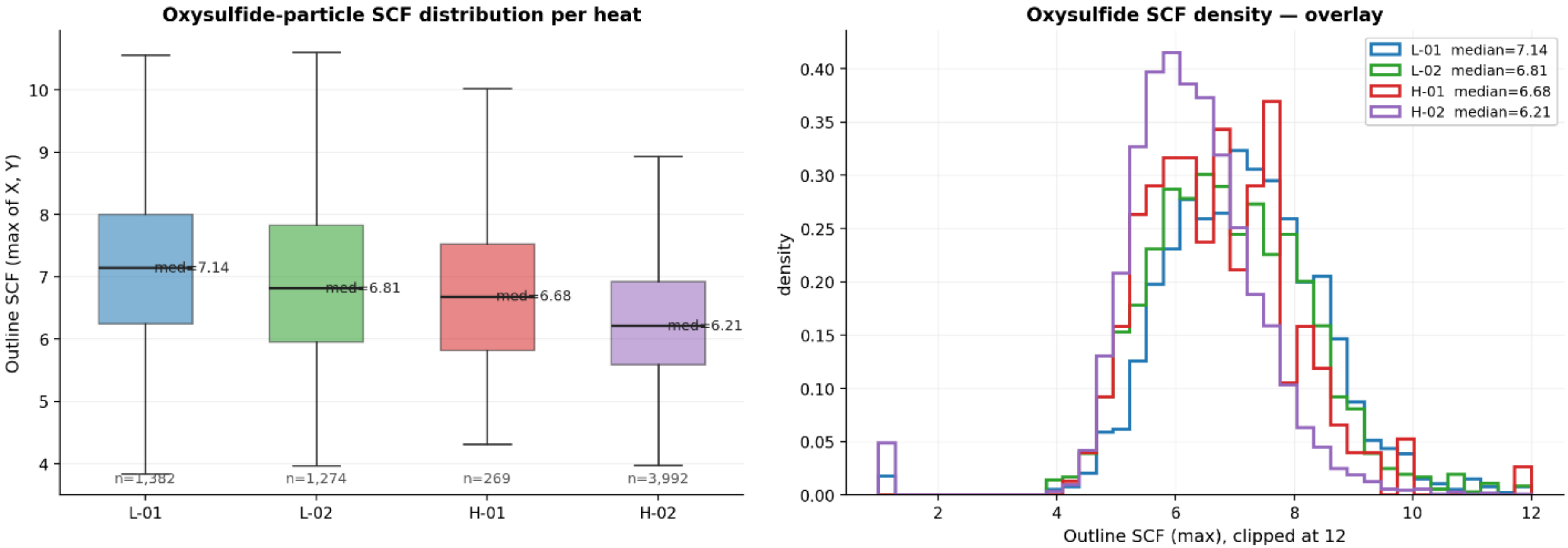



# Oxysulfide-particle SCF distribution

## per heat - L-01, L-02, H-01, H-02

*FEM-derived Outline SCF on OXYSULFIDE inclusions only (O ≥ 5 wt% AND S ≥ 5 wt%). Box: IQR + median; right panel: density overlay (clipped at SCF=12).*

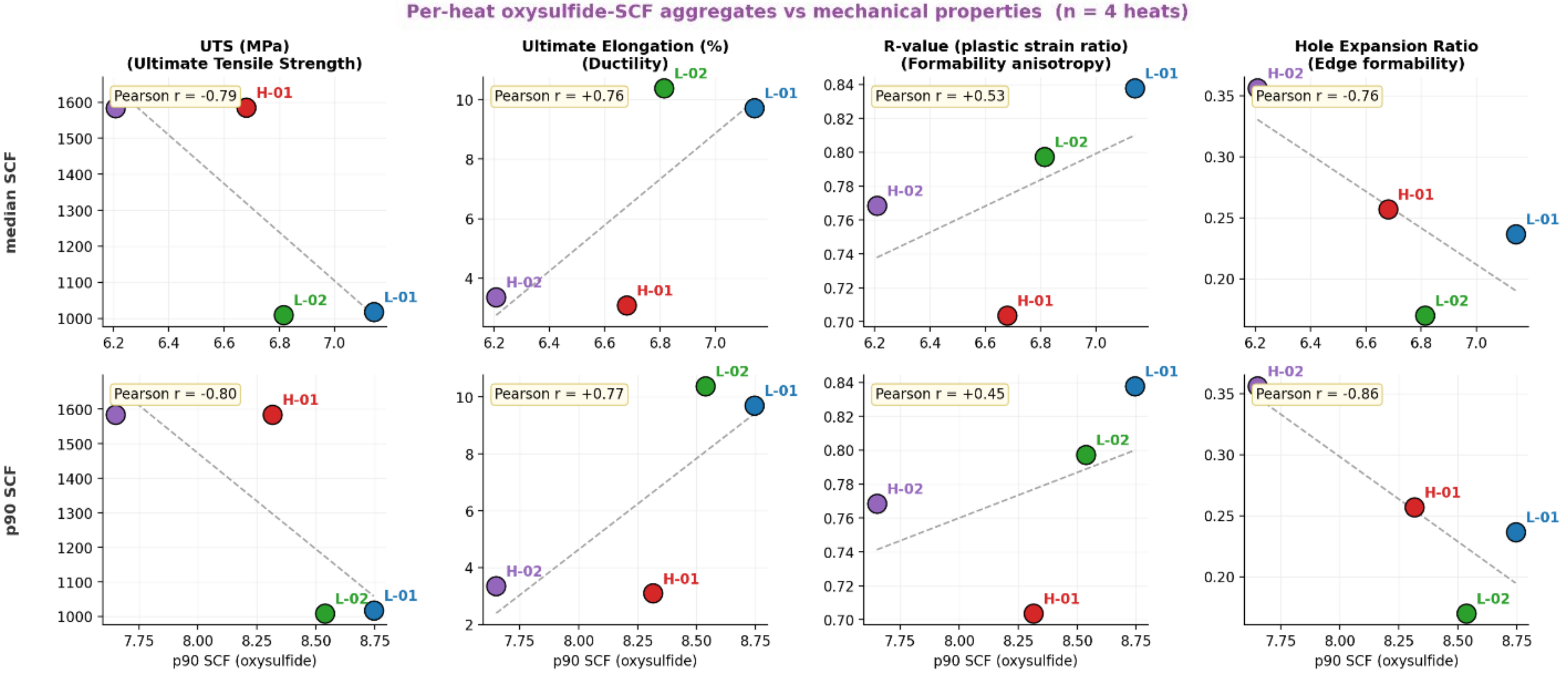
**Stress-concentration factor on OXYSULFIDE inclusions (O ≥ 5 wt% AND S ≥ 5 wt%)**



# Oxysulfide-SCF aggregates vs mechanical properties

## (per heat)

*Each point = one heat (mean of specimens for the y-axis property). Top row: median SCF vs UTS / Elongation / R-value / HER. Bottom row: same with p90 SCF on x-axis. Pearson r shown per panel (n = 4).*




OXYSULFIDE inclusions only (O ≥ 5 wt% AND S ≥ 5 wt%). SCF = max(Outline_SCF_X, Outline_SCF_Y). Mech values = mean of all available specimens per heat. n = 4 — Pearson r is directional only.

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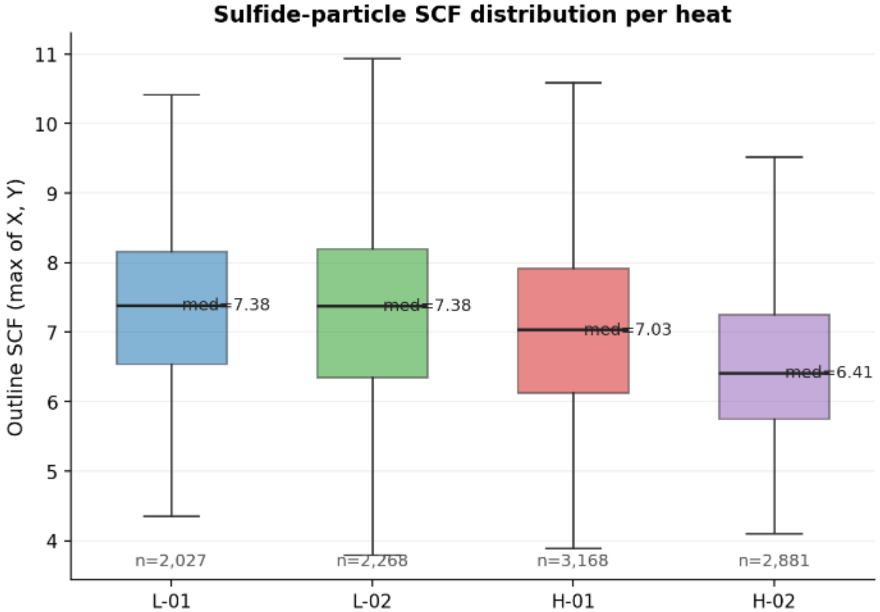
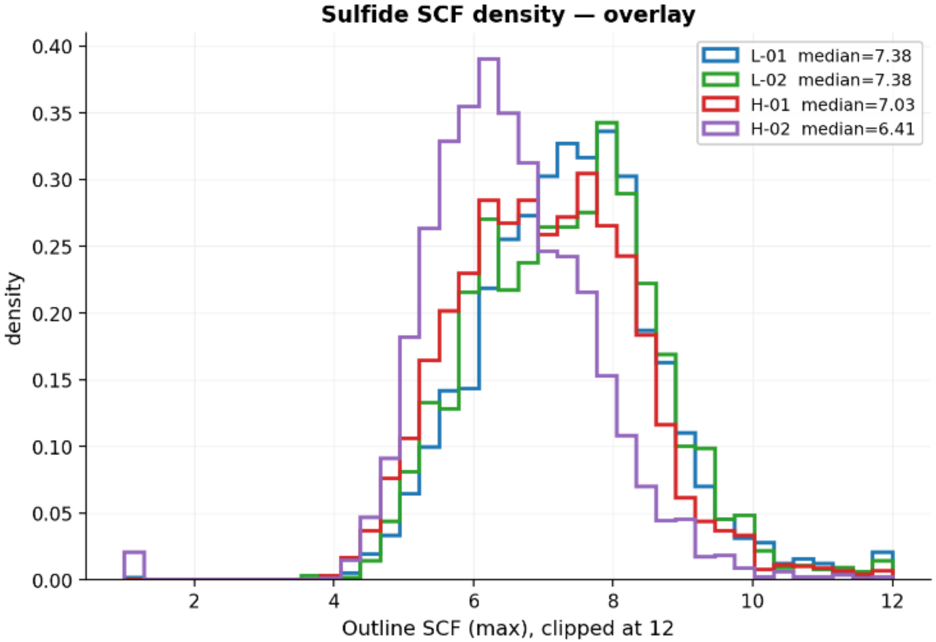
# Sulfide-particle SCF distribution per heat
## — L-01, L-02, H-01, H-02

*FEM-derived Outline SCF on SULFIDE inclusions only (O < 5 wt% AND S ≥ 5 wt%). Box: IQR + median; right panel: density overlay (clipped at SCF=12).*

**Stress-concentration factor on SULFIDE inclusions (O < 5 wt% AND S ≥ 5 wt%)**



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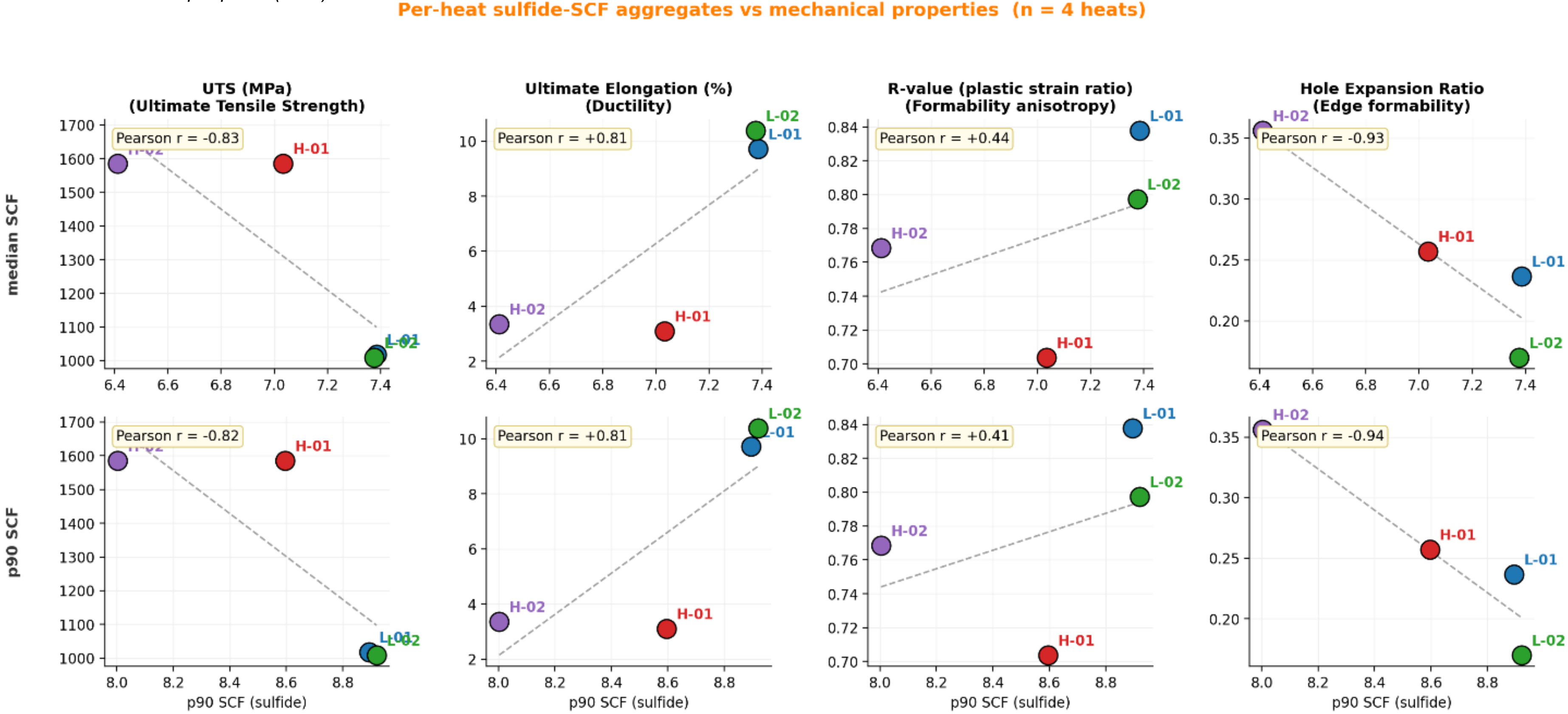
# Sulfide-SCF aggregates vs mechanical properties (per heat)

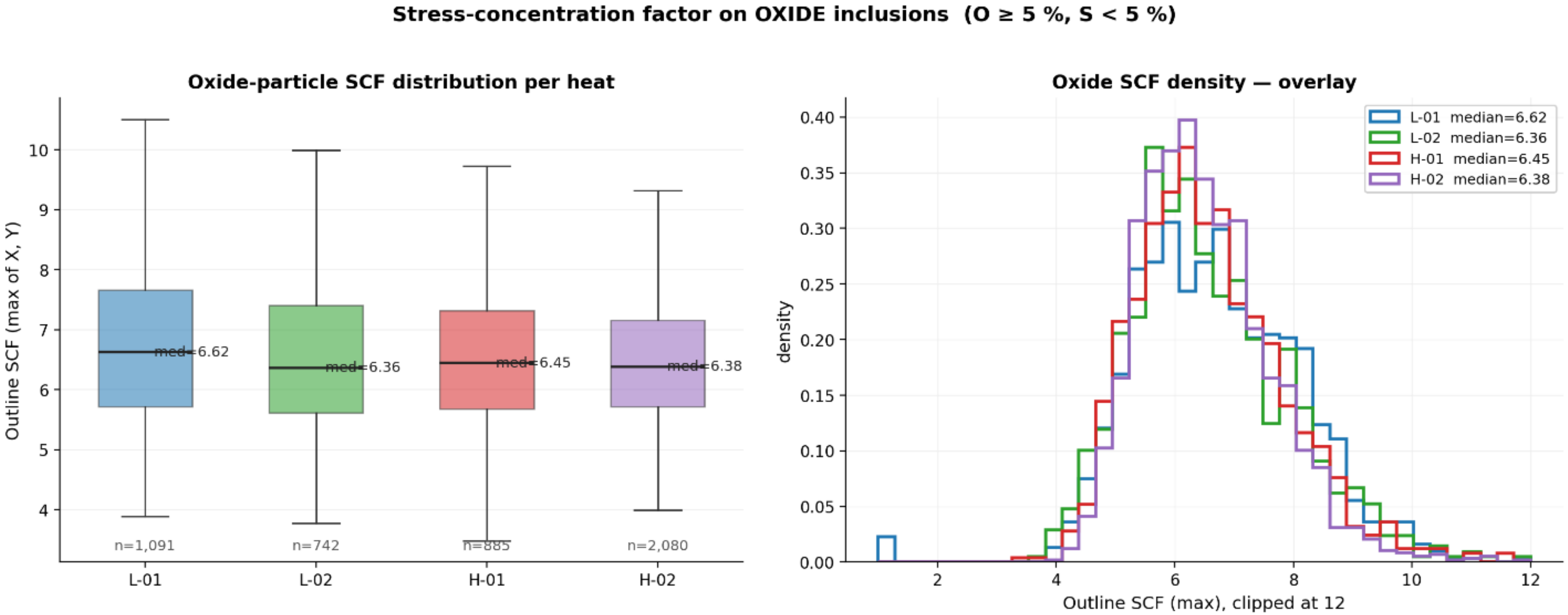
*Each point = one heat (mean of specimens for the y-axis property). Top row: median SCF vs UTS / Elongation / R-value / HER. Bottom row: same with p90 SCF on x-axis. Pearson r shown per panel (n = 4).*




SULFIDE inclusions only (O < 5 wt% AND S ≥ 5 wt%). SCF = max(Outline_SCF_X, Outline_SCF_Y). Mech values = mean of all available specimens per heat. n = 4 — Pearson r is directional only.

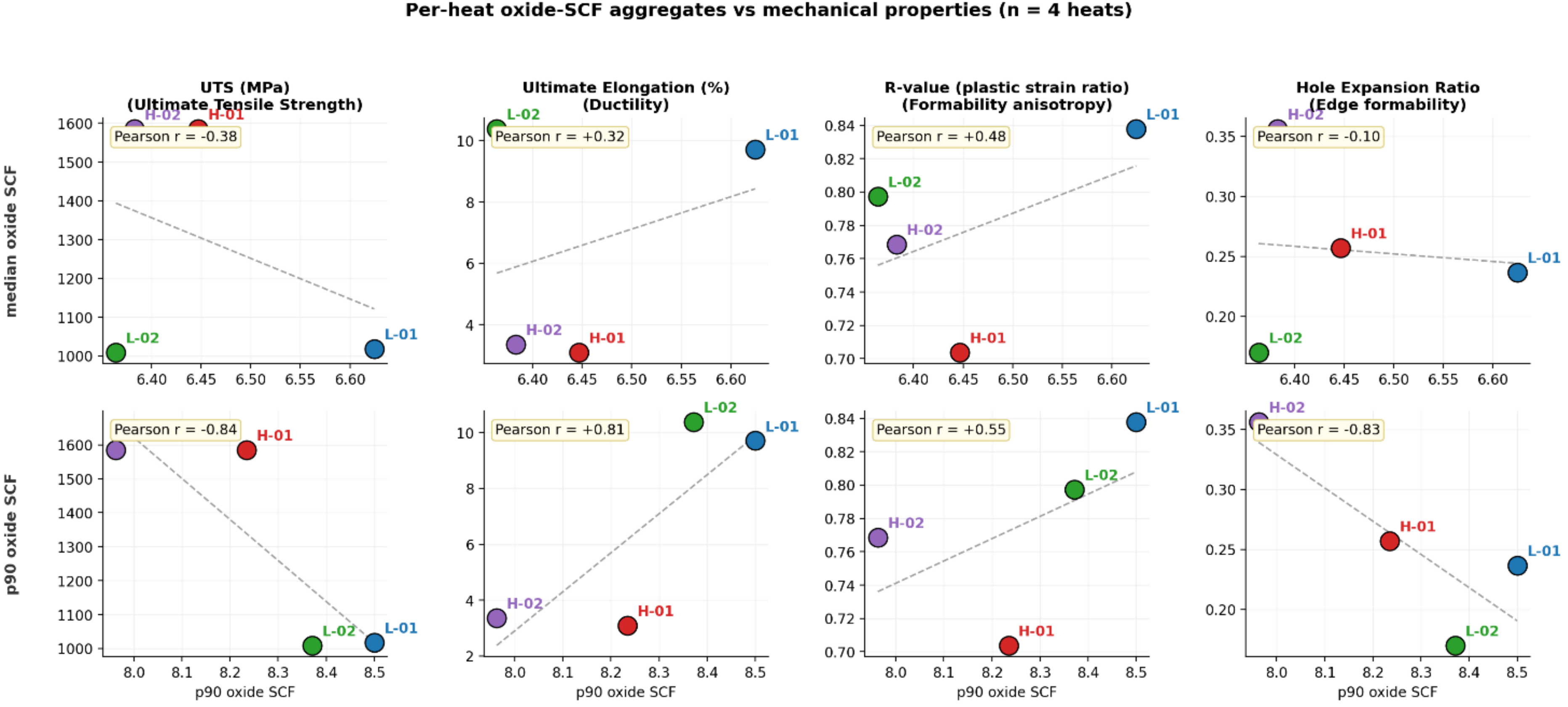
# Oxide-particle SCF distribution per heat - L-01, L-02, H-01, H-02

*FEM-derived Outline SCF on OXIDE inclusions only (O ≥ 5 wt%, S < 5 wt%). Box: IQR + median; right panel: density overlay (clipped at SCF=12).*



# Oxide-SCF aggregates vs mechanical properties (per heat)

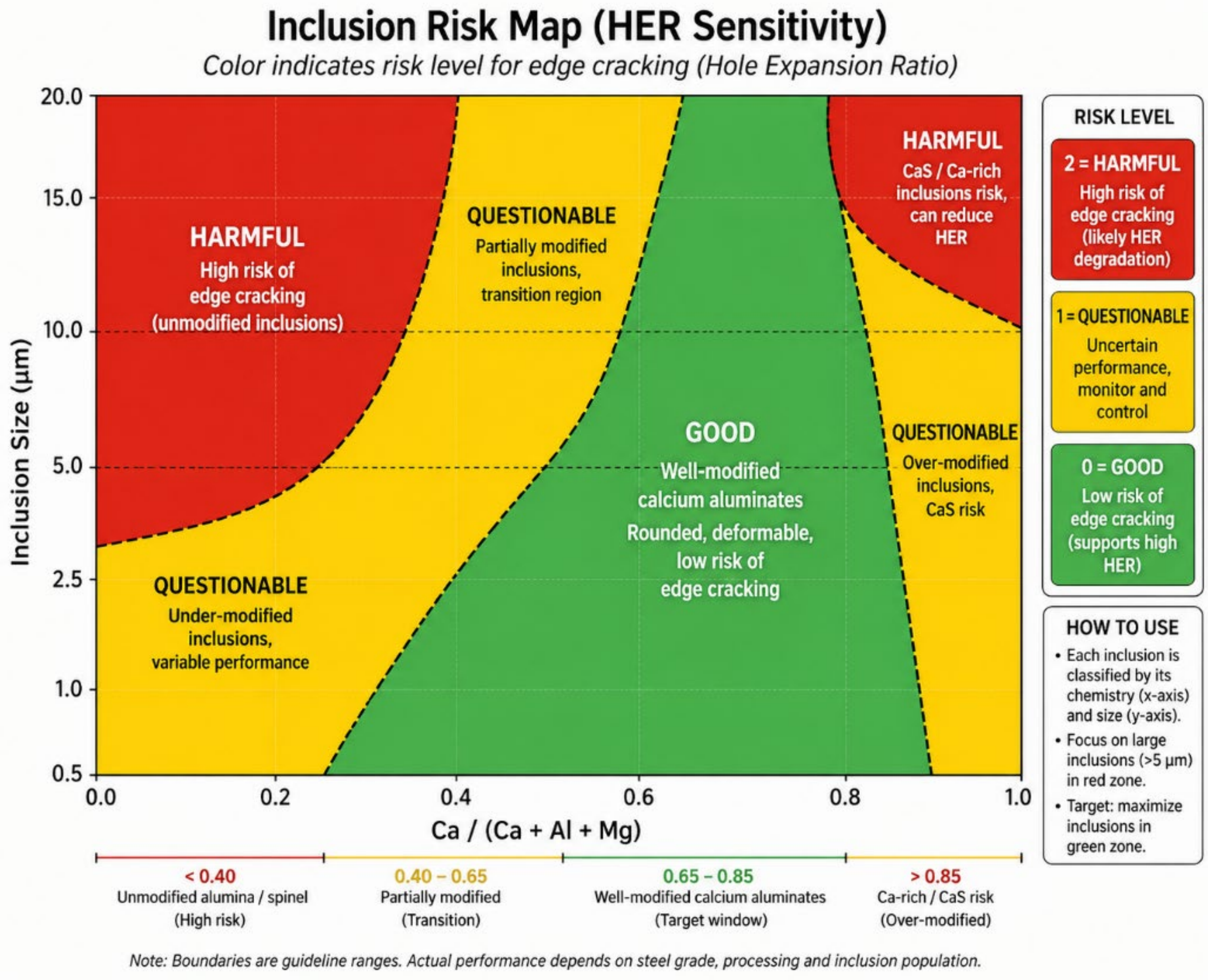
*Each point = one heat (mean of specimens for the y-axis property). Top row: median oxide SCF vs UTS / Elongation / R-value / HER. Bottom row: same with p90 oxide SCF on x-axis. Pearson r shown per panel (n = 4).*




OXIDE inclusions only (O ≥ 5 wt%, S < 5 wt%). SCF = max(Outline_SCF_X, Outline_SCF_Y). Mech values = mean of all available specimens per heat. n = 4 — Pearson r is directional only.

# Effect of Inclusion Chemistry on Mechanical Properties

| | UTS | Elong | R-value | HER |
|---|---|---|---|---|
| **Oxide median** | -0.38 | +0.32 | +0.48 | -0.10 |
| **Oxide p90** | -0.84 | +0.81 | +0.55 | -0.83 |
| **Oxysulfide median** | -0.79 | +0.76 | +0.53 | -0.76 |
| **Oxysulfide p90** | -0.80 | +0.77 | +0.45 | -0.86 |
| **Sulfide median** | -0.83 | +0.81 | +0.44 | -0.93 |
| **Sulfide p90** | -0.82 | +0.81 | +0.41 | -0.94 |


Inclusion Risk Map (HER Sensitivity)
Color indicates risk level for edge cracking (Hole Expansion Ratio)
20.0
15.0
10.0
5.0
2.5
1.0
0.5
Inclusion Size (µm)
0.0
0.2
0.4
0.6
0.8
1.0
Ca / (Ca + Al + Mg)
HARMFUL
High risk of edge cracking (unmodified inclusions)
QUESTIONABLE
Partially modified inclusions, transition region
HARMFUL
CaS / Ca-rich inclusions risk, can reduce HER
QUESTIONABLE
Under-modified inclusions, variable performance
GOOD
Well-modified calcium aluminates
Rounded, deformable, low risk of edge cracking
QUESTIONABLE
Over-modified inclusions, CaS risk
RISK LEVEL
2 = HARMFUL
High risk of edge cracking (likely HER degradation)
1 = QUESTIONABLE
Uncertain performance, monitor and control
0 = GOOD
Low risk of edge cracking (supports high HER)
HOW TO USE
• Each inclusion is classified by its chemistry (x-axis) and size (y-axis).
• Focus on large inclusions (>5 µm) in red zone.
• Target: maximize inclusions in green zone.
< 0.40
Unmodified alumina / spinel (High risk)
0.40 – 0.65
Partially modified (Transition)
0.65 – 0.85
Well-modified calcium aluminates (Target window)
> 0.85
Ca-rich / CaS risk (Over-modified)
Note: Boundaries are guideline ranges. Actual performance depends on steel grade, processing and inclusion population.

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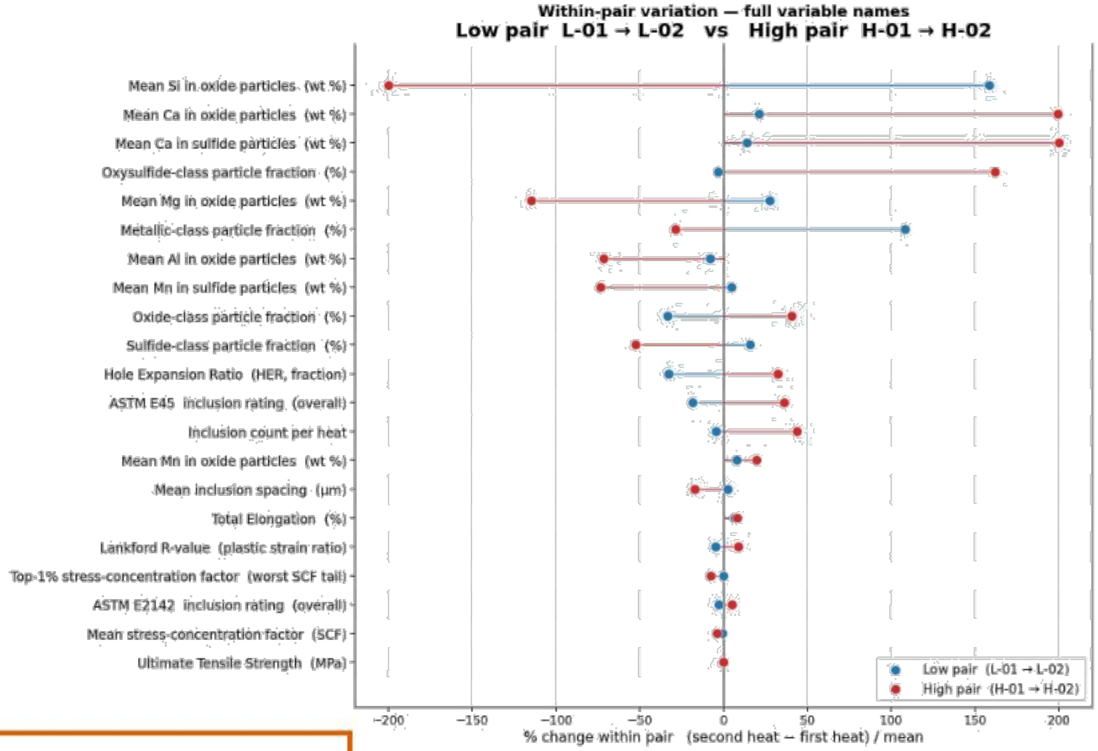
# Within-pair variation — full variable names

% change within pair (second heat − first heat) / mean. Blue = Low pair, Red = High pair.



# Property Covariation

| Feature | Δ Low (L-01 → L-02) | Δ High (H-01 → H-02) |
|---|---:|---:|
| oxide-cation Ca | +21% | +199% |
| sulfide-cation Ca | +14% | +200% |
| oxide-cation Al | −8% | −72% |
| oxide-cation Mn | +8% | +19% |
| Elongation | +7% | +8% |
| SCF top-1% | −0.2% | −8% |
| SCF mean | −1% | −4% |
| UTS | −0.8% | ~0% |

# Results and Analysis

- Identification of “worst fields” and stress hotspots
- Correlation between modeled stress and observed mechanical behavior
- Comparison of Cation Population with mechanical properties

“These results demonstrate directional, physically consistent relationships between inclusion characteristics and mechanical response; however, expanded datasets are required for predictive deployment.”

# Toward E45': A Next-Generation Standard

- ➢ Integrating AI, FEM, and inclusion population with mechanical properties provides conceptual framework for new predictive model
- ➢ Inclusion Cation ratios potential predictor of Steel Quality
    - o Potential for industry adoption and standardization

# Dr. Richard J. Lee

Chief Executive Officer
rlee@rjleegroup.com

RJ Lee Group

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