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14. ABSTRACT The objective of this STIR program was to utilize a data-analytics approach to predict the performance of an architecturally graded aluminum composite with a diffuse interface between alloys 5456 and 7055. The program supported the education and training of one graduate student pursuing a Masters of Science degree in Materials Science and Engineering. It was hypothesized that the compositional gradient would be primarily responsible for the performance of the composite system. To test this hypothesis a robust data framework was developed for spatially correlating disparate datasets for composition, microstructure, and hardness. This included open science					
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Report Title

Final Report: Interface effects of the properties and processing of graded composite aluminum alloys

ABSTRACT

The objective of this STIR program was to utilize a data-analytics approach to predict the performance of an architecturally graded aluminum composite with a diffuse interface between alloys 5456 and 7055. The program supported the education and training of one graduate student pursuing a Masters of Science degree in Materials Science and Engineering. It was hypothesized that the compositional gradient would be primarily responsible for the performance of the composite system. To test this hypothesis a robust data framework was developed for spatially correlating disparate datasets for composition, microstructure, and hardness. This included open-science protocols for data and metadata collection for energy dispersive X-ray spectrometry (EDS), X-ray photoelectron spectroscopy (XPS), electron backscatter diffraction (EBSD), and microhardness. Structural equation modeling was used to assess the statistical validity of mapping functions that predict performance at a particular position in the compositional gradient. The predictive capabilities of the derived mapping functions were then validated against a second, spatially sparse dataset. The analysis indicated that the large deviation in the hardness measurements made it difficult to produce functional forms that predict performance with R2 values greater than 0.61.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received

Paper

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Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

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Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Amit V. Kumar, Roger H. French, Jennifer L.W. Carter Study of Aluminum Graded Composies Using Data-Analyitics to Probe in Material Measures Governing Performance, (April 2015), CWRU Research ShowCASE.

Number of Presentations: 1.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	Discipline
Amit K. Verma	1.00	
FTE Equivalent:	1.00	
Total Number:	1	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Jennifer L.W. Carter	0.05	
FTE Equivalent:	0.05	
Total Number:	1	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:..... 0.00

Names of Personnel receiving masters degrees

<u>NAME</u>
Total Number:

Names of personnel receiving PHDs

<u>NAME</u>
Total Number:

Names of other research staff

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See Attachment

Technology Transfer

ABSTRACT

The objective of this STIR program was to utilize a data-analytics approach to predict the performance of an architecturally graded aluminum composite with a diffuse interface between alloys 5456 and 7055. The program supported the education and training of one graduate student pursuing a Masters of Science degree in Materials Science and Engineering. It was **hypothesized** that the compositional gradient would be primarily responsible for the performance of the composite system. To test this hypothesis a robust data framework was developed for spatially correlating disparate datasets for composition, microstructure, and hardness. This included open-science protocols for data and metadata collection for energy dispersive X-ray spectrometry (EDS), X-ray photoelectron spectroscopy (XPS), electron backscatter diffraction (EBSD), and microhardness. Structural equation modeling was used to assess the statistical validity of mapping functions that predict performance at a particular position in the compositional gradient. The predictive capabilities of the derived mapping functions were then validated against a second, spatially sparse dataset. The analysis indicated that the large deviation in the hardness measurements made it difficult to produce functional forms that predict performance with R^2 values greater than 0.61.

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STATEMENT OF THE PROBLEM

The proposed research focused on how architectural gradients (i.e., gradients in composition and microstructure) in a diffuse-interface composite, control its subsequent gradients in performance. The program fits into a larger goal of being able to design optimal architectural gradients for manufacturability and/or functional performance. To accomplish both the program goal and this long-term goal, the research team focused on a data-analytics approach to utilize quantifiable measures of architecture and performance to develop mapping functions that predict one measure from the other. From these mapping functions, new architectural gradients can be efficiently assessed and designed, thereby reducing development cost and time.

This study focused on a composite aluminum alloy with a diffuse interface. Produced by the Alcoa sequential casting process, the material has a gradient in composition from a stronger, precipitation strengthened alloy (7055) to a softer, strain-hardenable alloy (5456) [1], [2]. Alcoa donated material, 30x30x2 cm³ in volume. The material was cast, rolled and the surfaces finish ground following proprietary processing techniques. Therefore, the first step was quantifying the initial architectural gradients, followed by quantification of the performance gradients. Domain guided structural equation modeling was conducted to assess the statistically-significance different functional forms. The predictive capabilities of the mapping functions between local measures of architecture and performance were assessed with additional testing.

SUMMARY OF IMPORTANT RESULTS

Robust Data Framework

A major technical challenge of the program was to develop a framework to compare disparate datasets for composition, microstructure, and hardness. This was technologically challenging since each dataset had its own spatial resolution constraints. Utilizing the guidelines expounded by other researchers [3], we developed an open-source protocol for maintaining data and metadata associated the datasets pertinent for this program. The first result of this development was a protocol for cataloging the spatial locations of the different datasets such that local correlations could be explored and analyzed on datasets collected in a sequential fashion. Secondly, all metadata was collected and maintained in an open-source format (comma separated variables) to facilitate sharing of data and future analysis (beyond the scope of the program). When the results of the work are published, the data and meta-data will be made available either on a Git repository, a free and open source distributed version control system designed to handle small and large projects with speed and efficiency, maintained by the PI or on the journals supplementary materials site.

Exploratory Data Analysis

Exploratory Data Analysis (EDA) was conducted to visualize correlations between measures of composition and hardness conducted at six different locations along the compositional gradient. Pairwise-plots were utilized to visualize correlations between different measures and assessment the correlations were quantitatively done by fitting a linear mapping function, Figure 1. Pairwise-plots place the variables/measures along the diagonal of a square matrix, such that in each box below the diagonal is a visual representation of two variables along the diagonal, and the boxes above the diagonal are the r - and p -values from a linear mapping function fit between the variables. The variables for each data box are defined in the following manner: the y-axis of each box is determined by the variable listed on the same row as the box and the x-axis of each box is determined by the variable listed in the same column. As an example, data visualized in matrix location [5, 1] of Figure 1 has location along the gradient (location.z) visualized on the x-axis and magnesium concentration in wt% on the y-axis (Mg).

Visualization of the EDA indicates that as hypothesized the local performance of composite is a function of the compositional variables. The following results from the EDA can be used to simplify the variable space for the development of statistically validated mapping functions:

- Copper concentration does not vary with location (Figure 1: [6,1]) and as such does not show any correlation with the performance of the composite (Figure 1: [6,2]).
- Aluminum concentration is a redundant variable as there is a strong linear correlation between aluminum concentration and zinc concentration as indicated by an r -value of 0.96 and a p -value < 0.01 .

Therefore, we utilized variables of zinc and magnesium concentration to test functional forms for the mapping functions to predict location specific performance (hardness) from the measured composition.

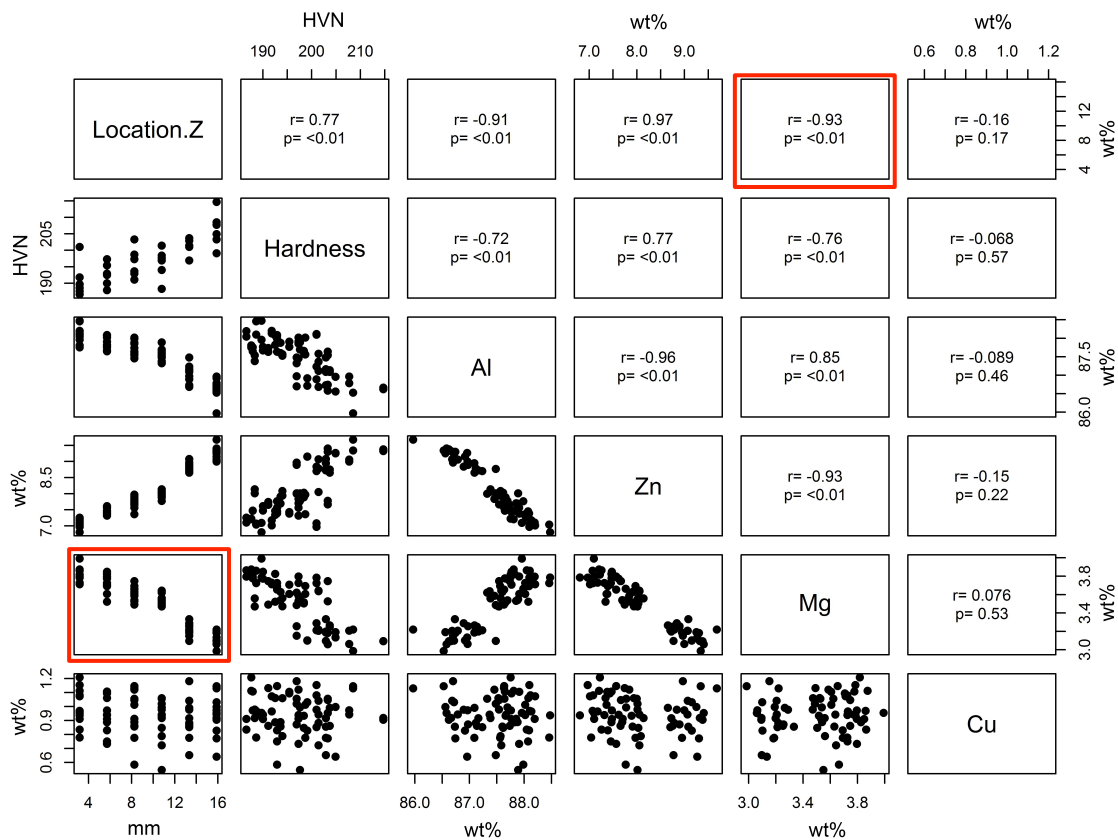


Figure 1. Pairwise-plot of correlations between performance (hardness) and mesostructure (wt% Al, Mg, Zn, Cu) measures. This shows that variations in spatial resolution between different data-collection techniques can be accounted for with responsible global origin definition. Visualized data and metrics of a linear fit for variables location.z and Mg concentration (matrix position [5,1]) are highlighted with a red box for ease of interpretation.

Mapping Function Development

Structural equation modeling was used to assess the statistical validity of mapping functions for one-to-one correlations between composition (Zn, and Mg concentration) and hardness. Seven different functional forms were assessed: simple linear, quadratic, simple quadratic, exponential, logarithmic, linear change point, and nonlinearizable exponential [4]. The

functional forms with the best fit are shown in Figure 2. The R^2 values for these one-to-one correlations, as well as visualization in the EDA (Figure 1 [i,2]) indicate that the spread in the performance data (hardness) makes it difficult to get good correlation between variables. It can also be seen that the functional forms that predict performance based on the two compositional variables is different. A logarithmic functional form best describes the correlation between Mg concentration and hardness, and as simple quadratic best describes the correlation between Zn concentration and performance. This might be expected since these two compositional variables are independent and strength the material is dependent by two different mechanisms (i.e., Zn: precipitation hardening, and Mg: solute strengthening).

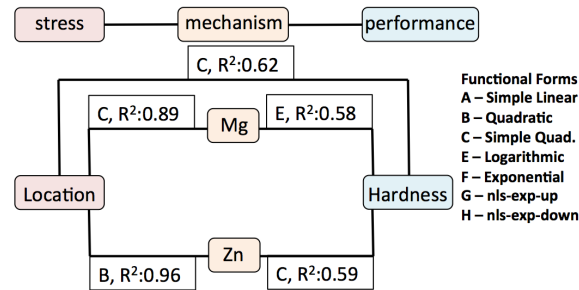


Figure 2. Visualization of the best functional forms for one-to-one correlations between stress-mechanism-performance. For implementation of these functional forms into a Finite Element Analysis, you would first utilize the functional forms to describe composition as a function of location along the gradient and then describe the performance in terms of the functional forms between composition and hardness.

Additionally, a combinatorial model where the separate one-to-one correlations were added in a simple summation was evaluated. Statistical analysis indicates that the following functional form provided similar fit of the performance predicted by one-to-one correlations of compositional values with an R^2 value of 0.61.

$$\text{Hardness}(x,z) = 218.3128 + 0.2335 * \text{Zn}(x,z)^2 - 29.0424 * \log(\text{Mg}(x,z))$$

Mapping Function Predictions

The predictive capability of the combinatorial functional form was assessed by collecting data at fewer spatial intervals on a new sample. Figure 3 shows a comparison between the measured hardness values, and the predicted hardness values based on measurements of the Mg and Zn concentrations. Additionally, the reverse correlations could be used to predict composition based on the hardness measurements.

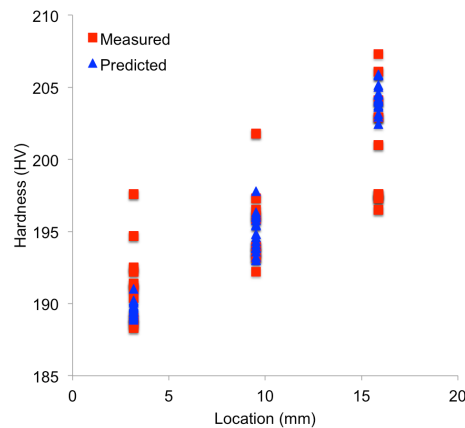


Figure 3. Combinatorial model predictions of the local performance based on compositional measurements compared to measured hardness measurements. The model predictions are within the natural standard deviation in the measured performance.

EBSD was used to assess the variations in the grain size and texture between the two extremes in the microstructure. It can be seen in Figure 4 that there is a significant difference in the grain size of at the two extremes of the microstructure, based on the available data it is still unclear if there is a systematic variation in texture. It was determined that metrics for these variables would also be necessary to fully model the performance of this material. The large grain size exhibited at both extremes of the microstructure could be the root cause of the variability in the hardness data. Therefore, it is still unclear if adding mapping functions between variables of grain size and hardness would significantly increase the predictive capabilities of the models due to the variable in performance as measured by the hardness measurements.

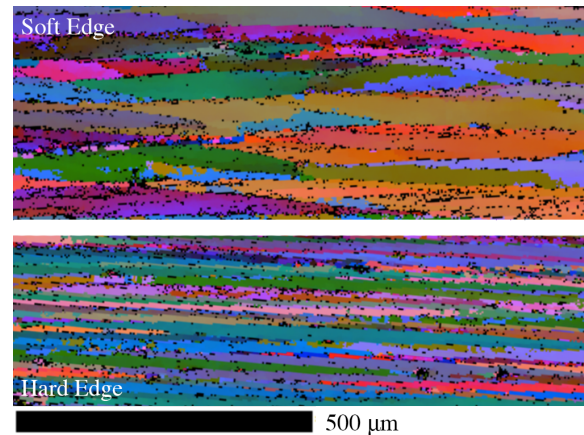


Figure 4. EBSD from the two extremes of the gradient, showing a systematic variation in grain size along the compositional gradient.

LEVEL OF EFFORT

It was originally proposed that a post-doctoral researcher would be responsible for accomplishing the tasks outlined in the program. Due to visa issues it wasn't possible to get a postdoctoral researcher in place prior to the start of the program. Instead, tasks were assigned to a first year graduate student working on their Masters of Science degree as a step towards competing a Ph.D. program in Materials Science and Engineering. The results of this STIR program will compose the thesis of work that the student submits as part of the Masters of Science program in Materials Science and Engineering during the Spring of 2016.

During the nine-month period we accomplished Tasks 1 and 3, and some of Task 2 as listed in the proposed Gantt Chart, Table 1. The development of the EDS and EBSD data collection protocols took more time than anticipated. Additional, no time for training on the R-analytics package was allocated and this required lead time before Task 3 could be accomplished. The PI and the graduate student are working to accomplish the unfinished tasks of this program. The results of this STIR will be prepared and submitted for publication in the near future to Materials Science and Engineering A, or Metallurgical and Materials Transactions A.

Table 1. Initial tasks proposed for this program. Tasks highlighted in blue were accomplished.

Task 1: Architecture Quantification
EDS/EBSD
Task 2: Performance Quantification
Sample Preparation
Hardness Testing
Pattern Development
Compression/Tension
Task 3: Data-Analytics
Study Design
Data Framework
Mapping Function
Task 4: Finite Element Analysis
Training
Architectural Gradient Functions
Mapping Functions
Validation

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