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Cooperative Research and Development Agreement Final Report

CRADA TC02406

February 8, 2024

Dr. Victor Castillo, AI-Driven Accelerated Inclusion Analysis for Energy Efficient Steelmaking

Innovations and Partnerships Office

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AI-Driven Accelerated Inclusion Analysis for Energy Efficient Steelmaking

Cooperative Research and Development Agreement Final Report
CRADA No. TC02406
Date Technical Work Ended: February 8, 2024

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A. Parties

This project was a relationship between Lawrence Livermore National Security, LLC and ArcelorMittal USA Research LLC.

Lawrence Livermore National Security, LLC
Lawrence Livermore National Laboratory
7000 East Avenue
Livermore, CA 94550

Vic Castillo, L-153
Tel: (925) 424-5049
Email: castillo3@llnl.gov

Yeping Hu, L-224
Email: hu25@llnl.gov

ArcelorMittal USA Research LLC
3001 E. Columbus Drive
East Chicago, IN 46312

Bernard Chukwulebe
Tel: (219) 256-7760
Email: bernard.chukwulebe@arcelormittal.com

Dr. Tathagata Bhattacharya, Project Manager
Tel: (219) 256-7687
Email: tathagata.bhattacharya@arcelormittal.com

This project is sponsored under the High-Performance Computing for Energy Innovation ("HPC4EI") Program of the Department of Energy's Advanced Materials & Manufacturing Technologies Office ("AMMTO") within the Energy Efficiency and Renewable Energy ("EERE") Office.

Project funding table for CRADA:

	Year 1		
Funding Type	Funds-in	*In-kind	Totals
ArcelorMittal	$0	$75,000	$75,000
Dept. of Energy [EERE]	$300,000		$300,000
Totals	$375,000		$375,000
**Federal Administrative Charge (FAC)	$0		$0

B. Project Scope

This was a collaborative effort between Lawrence Livermore National Security, LLC (LLNS) as manager and operator of Lawrence Livermore National Laboratory (LLNL) and ArcelorMittal USA Research LLC ("ArcelorMittal" as the Participant), to use scanning electron microscopy (SEM) images, computer vision and machine learning methods, and high-performance computing to accelerate the inclusion analysis process of liquid steel so that new methods can be used for near-real time process control on the shop floor.

The project was originally designated as a 12-month project, and consisted of four major tasks and the following four deliverables:

Task	Deliverable	Responsible Party	Due Date
1	Dataset of inclusion and EDS spectra	ArcelorMittal	End of Month 2
2	Final validated model package	LLNL	End of Month 10
3	Updated IntelliSEM code containing validated model and memo documenting results of testing the updated IntelliSEM software	ArcelorMittal	End of Month 12
4	Final Report and Abstract	LLNL, with input from ArcelorMittal	Completion or termination date of this CRADA

All of the deliverables for this project were successfully completed on time.

There were no amendments or No-Cost Time Extensions associated with this project.

No tangible property was exchanged.

There are no outstanding liens.

C. Technical Accomplishments

Tools		Input	Output
Visualization	Embedding Projector	Image	3D Image Projection
	Interactive Ternary Plotter	Element%	Ternary Plot
Modeling	Inclusion Type Predictor	Image	Inclusion Class
	Inclusion Chemistry Predictor	Image	Element%

A python-based software, originally known as "ArcelorMittal_Inclusion" but will be known going forward as “AI Driven Inclusion Analysis of Steel (ADIAS)” was successfully developed to achieve the goal of steel inclusion analysis. The software is equipped with multiple functionalities and the tools are summarized in the table above. The data visualization tools feature the embedding projector and the interactive ternary plotter, while the modeling tools include the inclusion type predictor and inclusion chemistry predictor. The following subsections contain detailed descriptions of each tool.

C.1 Visualization Tools

The embedding projector processes a large dataset of steel inclusion images, generating a 3D projection through the utilization of image features extracted from convolutional neural network (CNN) models. The results of this projection are illustrated in Figure 1. This projection can help visualize the intrinsic structure of the dataset, thereby enhancing the fundamental comprehension of the images and various inclusion classes. Various filters can be applied to facilitate the visualization of images sharing common inclusion class, project, sample, etc. In subsequent versions, additional filters can be included such as plant, specific process route, grade, and other key properties.

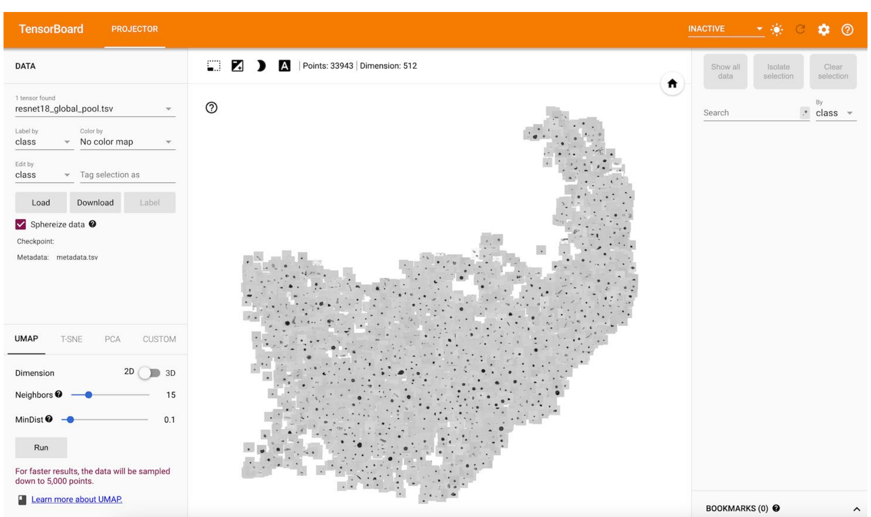

Figure 1. 3D embedding projection of steel inclusion images.

In addition to the embedding projector, the toolkit contains an interactive ternary plotter designed for visualizing the chemistry of steel inclusions across various inclusion types. As depicted in Figure 2, users can select targeting ternary elements and the plot is generated for the entire dataset, with data points colored based on their inclusion class. In future applications, this tool holds the potential for comparing predicted elemental distribution against the actual elemental distribution.

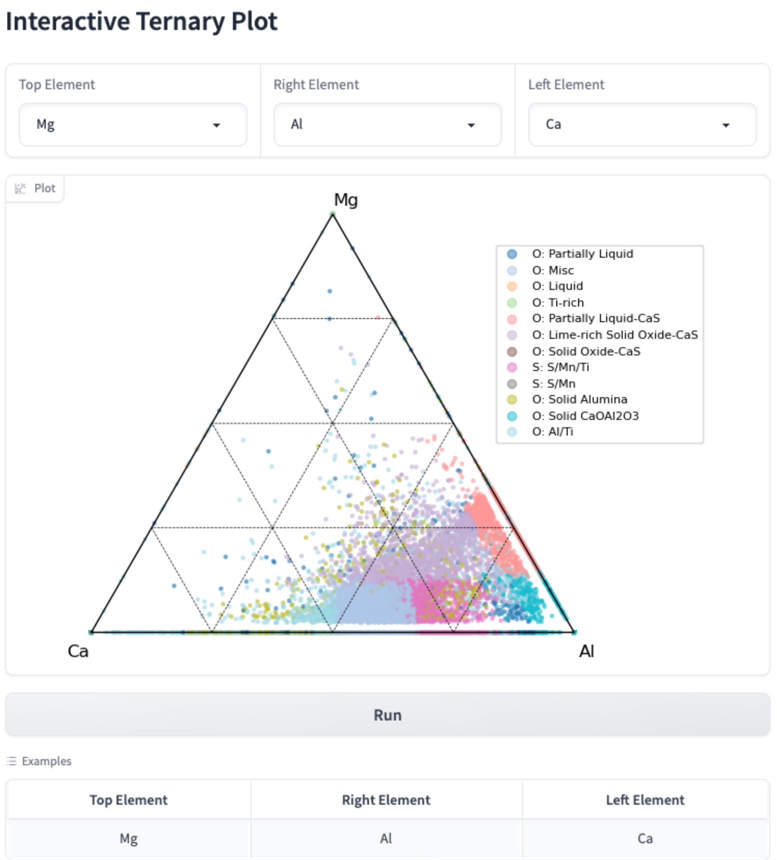

Figure 2. A ternary plot showing relative chemistry for steel inclusion images. Selected elements are Mg, Al and Ca.

C.2 Modeling Tools

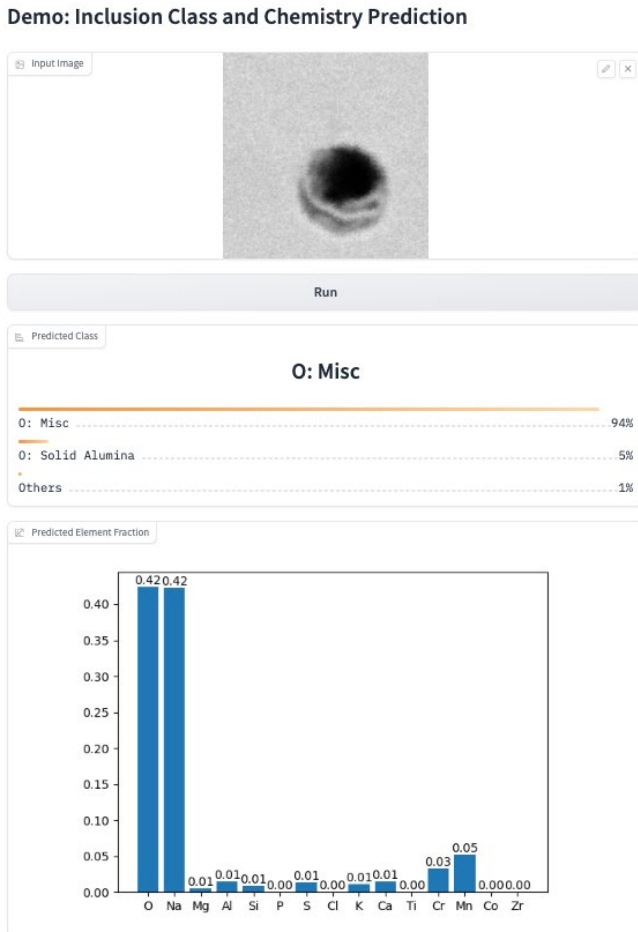

Figure 3. A Graphical User Interface for inclusion type predictor and inclusion chemistry predictor.

The modeling tools we designed have the capability to predict both the inclusion class and inclusion chemistry. Through the utilization of High-Performance Computing (HPC) resources, we conducted a systematic exploration of various deep learning models. Among them, ResNet, a convolutional neural network, emerged as the optimal choice, demonstrating a 60.8% accuracy in inclusion classification and achieving a mean absolute error (MAE) of 2.6% for element percentage prediction. Our implementation incorporates a user-friendly Graphical User Interface, as depicted in Figure 3, allowing users to upload an inclusion image for predicting both the inclusion class and chemistry. Moreover, we introduced an innovative model based on graph neural networks (GNN), which yielded a 59.3% accuracy in inclusion classification. In future advancements, augmenting the dataset and incorporating advanced machine learning models has the potential to further improve model performance. Additionally, delving into uncertainties will offer users insights into the reliability of predictions.

A notable challenge in our modeling approach is the significant diversity of classes within the dataset, where images of different inclusion types may closely resemble one another. Effectively addressing this challenge requires a thorough examination to devise an improved labeling strategy, ultimately resulting in a more accurate and efficient tool. Another challenge lies in the imbalanced distribution of data across different classes, necessitating a detailed evaluation and careful selection of training data for the prediction models.

D. Expected Economic Impact

D.1 Specific Benefits

Benefits to DOE
This CRADA was co-sponsored under the High-Performance Computing for Manufacturing (HPC4Mfg) Program of the Department of Energy's Advanced Materials & Manufacturing Technologies Office (AMMTO) within the Energy Efficiency and Renewable Energy (EERE) Office. LLNL was the lead Lab for the HPC4Mfg Program. This benefits the DOE by directly supporting the mission of the EERE AMMTO through its HPC4Mfg program. This CRADA was selected for this program by the DOE. This project advances the goals of the HPC4Mfg program by leading to reduced carbon emissions across the industrial steel manufacturing sector by improving efficiency and quality, saving energy, reducing waste, and ultimately reducing CO2. Also, this project allows LLNL to exercise their expertise in HPC, computer vision, and machine learning. Developing artificial intelligence (AI) methods to identify and control specific defects in metal processing is extremely important to the NNSA and AMMTO missions.

Benefits to Industry
This project will improve quality of steel, reduce cost for steel production, and reduce CO2 emissions. According to the Participant's approved HPC4EI proposal, yield losses of 1-2% can be attributed to harmful inclusions/particle entrapment during slab solidification from liquid steel. These losses, which are due to defective final products, reprocessing of intermediate products and yield loss at various processing steps, serve to reduce energy efficiency and productivity by significant amounts across the entire steel industry. In addition, to remake the lost yield, equivalent amount of greenhouse gas (GHG) emission is again incurred to the environment, resulting in double energy spending as well as increased GHG emissions (~ 6% of global GHG emissions come from the steel industry [13]). The total cost savings possible from a tiny reduction of 1% in yield loss for the whole U.S. steel industry is roughly $450 million/year, stemming from material, energy, labor, and other contributing items. Possible energy savings alone contribute greatly to this value, with nearly 15 PJ of energy savings per year equivalent to about 110 million gallons of gas savings, enough to power ~ 350,000 typical American homes for a year.

E. Participant Contribution

The results of this project, when completed, would be the first end-to-end industrial implementation of any HPC & AI-driven inclusion analysis workflow for the metal industry. The Participant intends to adopt the validated AI/ML models, once implemented through RJ Lee Group's IntelliSEM platform, as part of its day-to-day inclusion analysis and process troubleshooting. This CRADA supports ArcelorMittal in its mission to enhance its internal capabilities both in HPC expertise and AI/ML based advanced model developments. As part of ongoing digital transformation/smart manufacturing activities, ArcelorMittal Global R&D is in the process of expanding its modeling and simulation capabilities including adoption of HPC for industrial problem solving.

The Participant executed and delivered all project deliverables for Tasks 1 and 3. Additionally, the Participant met with the greater team biweekly and funded the RJ Lee Group's participation in the inclusion data pre-processing stage from their ASCAT/IntelliSEM system.

F. Documents/Reference List

Reports

Quarterly and Final progress reports were submitted to the HPC4EI program manager through the online reporting tool (https://proposalshpc4.inl.gov).

- Castillo_FY23Q2_Spring21_ArcelorMittal.doc
- Castillo_FY23Q3_Spring21_ArcelorMittal.doc
- Castillo_FY23Q4_Spring21_ArcelorMittal.doc
- Castillo_FY24Q1_Spring21_ArcelorMittal.doc

Additionally, we developed informal status reports that were presented and distributed at the biweekly team meetings.

Copyright Activity

A custom python-based software originally known as "ArcelorMittal_Inclusion" but will be known going forward as "AI Driven Inclusion Analysis of Steel (ADIAS)", (CP Number: CP02808) was developed by the LLNL team, reviewed for release by the LLNL ESW system, and distributed to ArcelorMittal USA Research LLC and their subcontractor, R.J. Lee Group. It contains the code for data analysis, visualization, and model development for inclusion composition detection.
This analysis software with a Graphical User Interface (GUI) was based on methods developed from the FY21 AMO ML Capability Project (Title: "Generalizable Scientific Machine Learning Tool Suite for Manufacturing"; Tracking ID: CAP-1-21-26488).

Subject Inventions

No Record of Invention was submitted for this CRADA.