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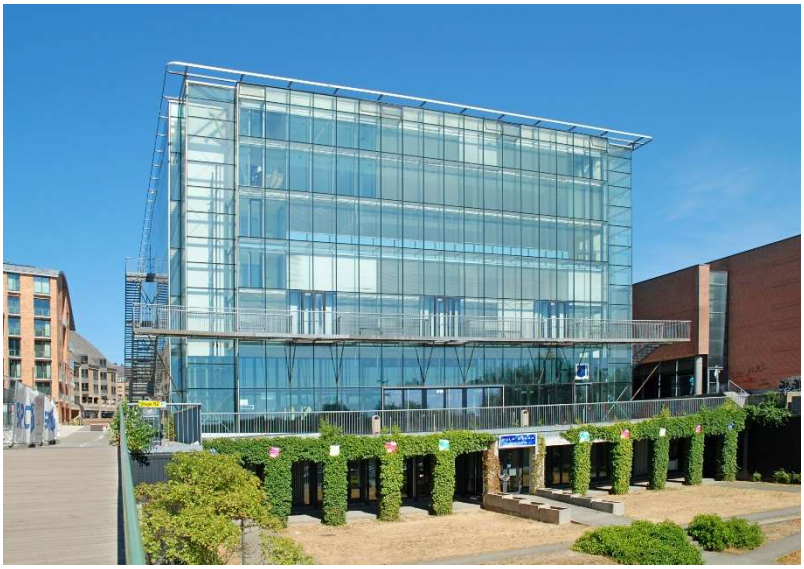
Machine Learning fro Micromechanics – First WG4 on-site workshop, February 22-23, 2024
Book of abstracts



UCLouvain, Louvain-la-Neuve, Belgium

Organizing Committee

Prof. Flavio Abreu Araujo (UCLouvain, Belgium)
Dr. Marie-Stéphane Colla (UCLouvain, Belgium)
Dr. Peter Ispanovity (Eötvös University, Hungary)
Dr. Peter Konijnenberg (Forschungszentrum Jülich, Germany)
Prof. Stefan Sandfeld (Forschungszentrum Jülich, Germany)

Practical informations

Meeting room

- Aula Magna, Place Raymond Lemaire 1, 1348 Louvain-la-Neuve, Belgium
- Room for Thrusday: « Foyer du Lac », on 3rd floor
- Room for Friday: « Foyer Royal », on 1st floor

Schedule

- Arrival in the meeting room from 1.15 pm on Thursday 22nd February
- End of the meeting at 3 pm on Friday 23rd February

Lunches

- Not included

Conference dinner

- Only for pre-registered participants
- On February 22nd, at 8.00 pm at restaurant Louvain House (same building and floor than for the Thrusday meeting room)
- Arrival on your own to the restaurant

Refunding

- Please have a look at the COST Travel Reimbursement Rules

MecaNano WG4 Machine Learning Kick-off Meeting in Louvain-la-Neuve

Thursday February 22, 2024

- 13:40 – **Introduction (Marie-Stéphane & Flavio)**
- 14:00 – **Tutorial 1** by **ANATOLE MOUREAUX**
- 15:00 – **Tutorial 2** by **Prof. Stefan SANDFELD**
- 16:00 – **Coffee break 1**
- 16:20 – Contributed talk 1 by **Tom Reclik**
- 16:40 – Contributed talk 2 by **Edoardo Rossi**
- 17:00 – Contributed talk 3 by **Peter Konijnenberg**
- 17:20 – Contributed talk 4 by **Mingdong Dong**
- 17:40 – Contributed talk 5 by **Erkan Ozkat**
- 18:00 – Contributed talk 6 by **Dénes Berta**
- 18:20 – Contributed talk 7 by **Ozgen Colak**
- 18:40 – Contributed talk 8 by **Burhanettin Erdem Alaca**
- 20:00 – **Networking Dinner**

Session 1 Chair: Prof. Flavio ABREU ARAUJO

Session 2 Chair: Prof. Stefan SANDFELD

Friday February 23, 2024

- 09:40 – **Welcome Coffee**
- 10:00 – **Tutorial 3** by **Dr. Julien LAM**
- 11:00 – **Tutorial 4** by **Prof. Gian-Marco RIGNANESE**
- 12:00 – **LUNCH**
  Participants are free to grab their meal in places in the city center (organizers will advise some places)
- 13:00 – Contributed talk 9 by **Pierre-Paul De Breuck**
- 13:20 – Contributed talk 10 by **Krzysztof Wieczerzak**
- 13:40 – Contributed talk 11 by **Nora Kovacs**
- 14:00 – Contributed talk 12 by **Ali Ercetin**
- 14:20 – **Closing words and discussion (Marie-Stéphane & Flavio)**
- 14:40 – **Coffee break 2**

Session 3 Chair: Prof. Flavio ABREU ARAUJO

Session 4 Chair: Dr. Peter Ispanovity

Tutorials

Anatole Moureaux
UCLouvain, Belgium

Surfing the AI wave: foundations, current feats, and future challenges

Since their first developments 80 years ago, the different techniques commonly referred to as 'Artificial Intelligence' have not stopped evolving. The field has known a remarkable diversification, leading to an ever-increasing number of applications in industry, research, health, and everyday life with impressive success. The development of high-performance computers with increased capabilities and the creation of new architectures and paradimgs has made AI more compelling than ever. Recently, the emergence of ChatGPT has brought AI to the forefront of the general public's attention. But what exactly is all that fuss about? Which techniques lie underneath the AI umbrella? What's under the hood of these famous neural networks, how do they work, and how can we use them? We will try to answer all these questions at the light of the last developments in the discipline. We will also have a look to a few of the most impressive feats of AI throughout history, as well as the future challenges ahead.

Prof. Stefan Sandfeld
Forschungszentrum Jülich, Germany

Introduction to Machine Learning and Data Science

This tutorial gives an introduction to the most important concepts and tools of machine learning and data science with particular emphasize on materials science. It starts with an overview of the most important notions and elucidates them based on small but concrete examples. The most important machine learning approaches and models are introduced, ranging from approaches for regression, classification, clustering. Last but not least, deep learning methods discussed which are particularly important for microscopy images.

Tutorials

Dr. Julien Lam
Chargé de recherches CNRS, Université de Lille

Atomistic simulations using machine-learning interaction potentials

Atomistic simulations have played a crucial role in the discovery of novel materials and the understanding of their specific properties. In this context, quantum calculations, including ab initio and density functional theory are the most accurate for calculating equilibrium properties and provide quantitative results comparable to experiments. In the meantime, empirical interaction potentials have also been employed to perform larger scale simulations yet with significantly lower accuracy, when compared to quantum calculations. In the past couple decades, machine-learning have been proposed as a way to bridge the gap between quantum accurate calculations and fast empirical modeling.
In this tutorial, we will give a short review on machine-learning interaction potentials describing the theoretical background before showing examples targeted to nanomaterial modeling.

Prof. Gian-Marco Rignanese
UCLouvain, Belgium

Materials process and property predictions from limited and multi-fidelity datasets

The available materials data are often rather limited. Unfortunately, typical machine-learning approaches generally require large amounts of data to make accurate predictions. To tackle this limitation, I will introduce MODNet, an all-round framework which relies on a feedforward neural network, the selection of physically meaningful features, and when applicable, joint-learning. Next to being faster in terms of training time, this approach is shown to outperform current graph-network models on small datasets.
Furthermore, materials data often present various levels of accuracy, with typically much less high- than low-fidelity data. I will present an approach to extract as much information as possible from all available data by improving the quality of the data through denoising.
Finally, I will discuss how active learning can be used to optimally perform data acquisition.

Oral contributions

Integrating Deep Learning Super-Resolution for Accelerated Analysis

Tom Reclik*[1]

[1]Institut für Metallkunde und Metallphysik (IMM) – RWTH Aachen, 52056 Aachen, Germany

Abstract

Performing high-resolution large-area scanning electron microscopy for the analysis of micro- and nanoscale features, poses significant challenges, including prolonged scanning durations and potential sample degradation due to extended electron beam exposure. This is further amplified, when the time dimension in in-situ experiments is added. Whereas we have automated the processof the analysis of large-area high-resolution micrographs using deep learning in the past, here we focus on accelerating the imaging process, by employing deep learning super-resolution algorithms coupled with the automated high-resolution rescanning of points of interest. Our approach significantly speeds up the imaging process, thereby enabling future studies of the time evolution of nano-mechanical processes in high-resolution with a high statistical relevancy.

*Speaker

High-Speed Nanoindentation Mapping and Machine Learning Synergy: Unraveling Phase Complexity in Advanced High Strength Steels

Federico Bruno[1], Georgios Kostantopoulos[2], Edoardo Rossi*[3], Gianluca Fiore[1], Costas Charitidis[2], Marco Sebastiani[3], Luca Belforte[4], and Mauro Palumbo[1]

[1]Università degli studi di Torino = University of Turin (UNITO) – Via Verdi, 8 10124 Torino Italie, Italy

[2]National Technical University of Athens [Athens] (NTUA) – Patission Complex, 42, Patission str, 10682 AthensZografou Campus - 9, Iroon Polytechniou str - 15780 Zografou, Athens, Greece

[3]Università degli Studi Roma Tre (ROMA TRE) – Via Ostiense, 133 - 00154 Rome, Italy

[4]Centro Ricerche Fiat (CRF) – Str. Torino, 50, 10043 Orbassano TO, Italy

Abstract

This study introduces a **machine learning-based methodology** to decipher the **complex phase compositions of Advanced High Strength Steels** (AHSS), particularly TRIP-assisted bainitic-ferritic (TBF) multiphase steels. The challenge lies in accurately identifying and quantifying phases like martensite, austenite, bainite, and ferrite, often indistinguishable due to similar crystal structures. Our approach synergizes **high-speed nanoindentation mapping** (HSNM) with **Electron Backscatter Diffraction** (EBSD) analysis, enhanced by sophisticated machine learning algorithms, to establish a **robust structure-property relationship at the nanoscale**. The methodology commences with machine learning-informed HSNM, employing the expectation-maximization algorithm to fit probability distributions of nanoindentation data. This step is pivotal in deriving primary mechanical phase statistics, enabling the correlation of elastic modulus and hardness with specific microstructures using nanoindentation data alone. Subsequently, a supervised machine learning approach refines this correlation, ensuring precise one-to-one mapping of EBSD and nanoindentation data through advanced image analysis and data clustering techniques. Further augmenting this protocol, machine learning is applied to analyze Inverse Polar Figure (IPF) mapping, respectively. This aids in understanding grain anisotropy and characteristics, while k-nearest-neighbors regression is employed for data imputation, addressing gaps in descriptors related to nanoindentation, grain boundaries, and EBSD phases. This integrated, data-driven approach not only overcomes the limitations of traditional SEM-EBSD analysis in phase distinction but also offers a reusable, modular framework. It represents a significant leap in the precise identification and quantification of various phases in AHSS, essential for advancing the design and application of these complex materials.

*Speaker

ML-based Analysis of Kikuchi Patterns

Peter Konijnenberg*[1] and Stefan Sandfeld[1]

[1]FZ Juelich (FZJ) – Wilhelm-Johnen-Straße, 52428 Jülich, Germany

Abstract

Electron BackScatter Diffraction (EBSD) is an analytical technique for scanning electron microscopy that is still rapidly evolving. On the software side, the core of this technique is formed by an algorithm to accurately and swiftly analyze electron diffraction images (Kikuchi patterns). Traditionally this is achieved in a 2-stage process of band detection by a Hough-transform and a consecutive band indexing by e.g. a triplet-voting approach. In the last decade some significant improvements were reported by so-called pattern matching algorithms that essentially cross-correlate the acquired patterns with forward-simulated patterns, see e.g. (1,2). Although, the application of neural networks (for verification of Hough-peaks) dates back quite some time ago (3), its application to the entire pattern analysis process was reported only relatively recently, see e.g. (4,5). Here, forward-simulated patterns are utilized to train a convolutional neural network (CNN), which then can be used for the task of analyzing acquired patterns.
We report about the development and application of such a ML-based approach to analyze Kikuchi patterns. Some significant differences to the classical Hough-based approach are explained, some pitfalls are elucidated, and the new approach is also benchmarked for its usability.

References:

1 Chen, Y. H., et al. *Microscopy and Microanalysis* 21.3 (2015): 739-752.

2 Hielscher, R., Bartel F., Britton, T.B. *Ultramicroscopy* 207 (2019): 112836.

3 Schwarzer, R.A., Sukkau, J. *Advanced Engineering Materials* 5.8 (2003): 601-606.

4 Dipendra, J. et al. *Microscopy and Microanalysis* 24.5 (2018): 497-502.
5 Ding, Z., Pascal, E., De Graef, M. *Acta Materialia* 199 (2020): 370-382.

*Speaker

Nanotribological Behavior of 2D materials by AFM

Mingdong Dong*[1]

[1]Aarhus University (AU) – Denmark

Abstract

Friction is a universal phenomenon with profound implications. This talk employs advanced AFM techniques to explore the frictional properties of two-dimensional (2D) materials and their interactions with small molecules. Our goal is to deepen the understanding of friction reduction and its underlying mechanisms, facilitating the development of innovative technologies.
Using atomic force microscopy (AFM) coupled with machine learning, we analyze the dynamic behavior of small molecules during sliding friction processes in various environments. Machine learning provides a sophisticated data analysis, revealing insights into the influence of small molecules on 2D material friction. Results show the impact on friction hysteresis in single-layer graphene and changes in lattice patterns and friction forces in transition metal dichalcogenides.

This study underscores the crucial role of machine learning in precise data analysis, emphasizing its significant contribution to understanding complex interactions. The findings presented pave the way for the development of advanced materials and lubrication technologies.

*Speaker

Fault detection in UAVs using time series data and deep learning

Erkan Ozkat*[1]

[1]Recep Tayyip Erdogan University (RTEU) – Department of Mechanical Engineering, Ataturk Cd, Rize, Turkey

Abstract

The application of deep learning methods for condition monitoring and failure diagnosis from vibration data has gained significant attention in various industries. Vibration data is often collected from machines and equipment to assess their health and detect potential faults or failures. Deep learning (DL) and Machine learning (ML) techniques, with their ability to automatically learn hierarchical representations from data, have shown promise in improving the accuracy of condition monitoring and failure diagnosis. Vibration data, viewed as time series data, plays a dual role in predictive analytics. It enables forecasting future behavior for proactive decision-making based on historical observations. Additionally, the time series nature facilitates anomaly detection, identifying deviations from normal patterns that may indicate faults. This integrated approach supports comprehensive condition monitoring and predictive maintenance, enhancing operational efficiency and minimizing downtime. In this study, spectrograms of vibration signals underwent Short Time Fourier Transform (STFT) for feature extraction, serving as input for training 1D Convolutional Neural Network (CNN). The application of STFT allows for the representation of time-varying frequencies in the vibration signals, capturing nuanced patterns essential for machine learning analysis. By employing 1D CNN, the research aims to forecast future values based on historical observations, allowing for better decision-making and planning, and to identify unusual patterns or events that deviate from the expected behavior in the time series.

*Speaker

Predicting stress response from acoustic emission with machine learning

Dénes Berta*[1], Balduin Katzer[2], Katrin Schulz[2], and Péter Ispánovity[1]

[1]Eötvös Loránd University (ELTE) – H-1053 Budapest, Egyetem tér 1-3, Hungary
[2]Karlsruhe Institute of Technology (KIT) – Campus North, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen / Campus South, Kaiserstraße 12, 76131 Karlsruhe, Germany

Abstract

In the micron and sub-micron scale, the plastic deformation of crystalline materials exhibits a complex behavior characterized by a series of random strain bursts. This phenomenon results in significant sample-to-sample variation in the plastic response within this size regime. It has also been observed that these deformation events are accompanied by acoustic emission (AE) signals (1). In this study, we endeavor to predict the stress response of compressed single crystalline Zn micropillars by leveraging machine learning (ML) techniques, utilizing simultaneously measured AE data. The investigated specimens demonstrate predominantly single-slip behavior, with dislocation avalanches in the basal plane being the dominant deformation mechanism. These avalanches lead to observable stress drops and concomitant AE signals, making the application of ML feasible. While prior studies have shown the predictability of coarse features in stress-strain curves in simple model systems (2), our focus here is on predicting the finer features. Our presentation demonstrates that ML can reasonably predict the fine structure of stress-time curves created by stress drops. We present the methods employed, their limitations, and discuss potential applications of our findings.
(1) Ispánovity, Péter Dusán, et al. "Dislocation avalanches are like earthquakes on the micron scale." Nature communications 13.1 (2022): 1975.
(2) Salmenjoki, Henri, Mikko J. Alava, and Lasse Laurson. "Machine learning plastic deformation of crystals." Nature communications 9.1 (2018): 5307.

*Speaker

MATERIAL PARAMETER DETERMINATION OF SIMPLIFIED COOPERATIVE VISCOPLASTICITY THOERY BASED ON OVERSTRESS FOR NANOCOMPOSITES USING GENETIC ALGORITHM OPTIMIZATION METHOD

Ozgen Colak*[1] and Yuksel Cakir[2]

[1]Yildiz Technical University (YTU) – YTU Makina Fak., Turkey
[2]Istanbul Technical University – Turkey

Abstract

Simplified cooperative-viscoplasticity theory based on overstress (C-VBO) theory is developed to cover the time, temperature, and graphene fraction dependent mechanical behavior of the nanocomposite material. To define the behavior of nanocomposites, the Mori-Tanaka homogenization scheme is used with C-VBO model. Graphene-epoxy nanocomposite materials are manufactured and mechanical characterization is performed. Following the mechanical characterization, the simplified C-VBO model is used to simulate rate-dependent uniaxial compression behaviors for different graphene fractions (0.1 and 0.5 wt.%). At this point, to determine the material parameters of the simplified C-VBO model for nanocomposites, genetics algorithm (GA) as a machine learning (ML) tool is used.
In recent decades, the use of ML techniques in the field of materials modeling has received significant attention due to their ability to analyze a vast amount of data and reveal correlations between several complex interrelated phenomena. GA which is based on a natural selection process that mimics biological evolution starts with chosen an arbitrarily population of individuals. The algorithm repeatedly modifies a population of individual solutions. The optimization procedure searches for the best individual by considering the fitness function in the population. GA optimization procedure was implemented by using MATLAB. The programs consist of GA optimization M-File for obtaining parameters and IMS Fortran scripts of the model.
Using the material parameters obtained from GA, the stress-strain behavior of graphene-epoxy nanocomposite under compression is plotted and good match with experimental data is depicted.

*Speaker

Interpretation of Scale Effect through Machine Learning: Atomistic Evaluation of Mechanical Behavior in Silicon Nanowires

Sina Zare Pakzad[1], Mohammad Nasr Esfahani[2], Demircan Canadinc[1], and B. Erdem Alaca*[1]

[1]Koç University – Rumelifeneri Yolu, 34450 Sarıyer-İstanbul, Turkey
[2]University of York – York YO10 5DD, UK, United Kingdom

Abstract

Nanowires play a pivotal role in different fields such as nanoelectromechanical systems, nanoelectronics, and energy applications. As nanowires decrease in size, their mechanical characteristics are increasingly influenced by surface attributes. This study examines the mechanical properties of silicon nanowires, with a specific emphasis on their modulus of elasticity. Using a comprehensive approach, the research integrates atomistic modeling through molecular dynamics simulations with advanced machine learning techniques. The molecular dynamics simulations generate a substantial dataset, surpassing 4000 data points, revealing the mechanical response of silicon nanowires. Exploring the partial dependencies between surface state and crystal orientation provides a methodology for estimating the modulus of elasticity in silicon nanowires. The research illustrates an insightful approach by showcasing how elasticity depends on orientation through the use of inverse pole figures. Furthermore, the study interprets the discrepancies associated with the scale effect that bridges the size-dependent modulus of elasticity of silicon nanowires between different efforts in the literature. Investigating the elastic properties of silicon nanowires (70-240 GPa), particularly in bottom-up nanowires, machine learning aids in understanding size-dependent effects. This analysis explores the transition of sub-20 nm silicon nanowires, considering standard deviation ranging between 10 to 15 GPa. Notably, the deviation decreases to a few GPa beyond 20 nm, unveiling important insights into effective parameters such as surface condition (native oxide) and computational factors. This methodology enhances our understanding of the mechanical properties of silicon nanowires and establishes a crucial link between computational and experimental research domains, laying the groundwork for advancements in nanoelectromechanical applications.

*Speaker

Pushing the boundaries of materials discovery through generative design

Pierre-Paul De Breuck*[1]

[1]Université catholique de Louvain (UCLouvain) – Belgium

Abstract

Conventional materials screening methods typically rely on supervised techniques to identify potential candidates from existing databases. However, the vast universe of functional materials extends far beyond our current knowledge, with many unknowns. Generative models present a new paradigm by generating entirely new compounds, which can also adhere to specific property constraints. In this presentation, I will provide a brief overview of generative models, with a focus on generative flow networks, and their role in crystal structure design. I will delve into their promising potential while also addressing the inherent limitations in the context of materials science.

*Speaker

Unlocking the potential of CuAgZr metallic glasses: A comprehensive exploration with combinatorial synthesis, high-throughput characterization, and machine learning

Krzysztof Wieczerzak*[1]

[1]Laboratory for Mechanics of Materials and Nanostructures [Thun] (EMPA) – Feuerwerkerstrasse 393602 Thun, Switzerland

Abstract

In this work, we investigate the CuAgZr metallic glasses (MGs), a promising material for biomedical applications due to their high strength, corrosion resistance, and antibacterial activity. Using an integrated approach of combinatorial synthesis, high-throughput characterization, and machine learning, we efficiently explored the mechanical properties of CuAgZr MGs. The investigation found that post-deposition oxidation in inter-columnar regions with looser packing causes high oxygen content in Cu-rich regions, significantly affecting the alloys' mechanical behavior. The study also revealed that nanoscale structural features greatly impact plastic yielding and flow in the alloys. Machine learning algorithms were tested, and the multi-layer perceptron algorithm produced satisfactory predictions for the alloys' hardness of untested alloys, providing valuable clues for future research. Our work demonstrates the potential of using combinatorial synthesis, high-throughput characterization, and machine learning techniques to facilitate the development of new metallic glasses with improved strength and economic feasibility.

*Speaker

Physically Recurrent Neural Networks for Computational Homogenization of Composite Materials with Microscale Debonding

Nora Kovacs*[1], Marina Maia[1], Iuri Rocha[1], Carolina Furtado[2], Pedro Camanho[2], and Frans Van Der Meer[1]

[1]Delft University of Technology (TU Delft) – Postbus 5 2600 AA Delft, Netherlands
[2]Faculdade de Engenharia da Universidade do Porto (FEUP) – Rua Dr. Roberto Frias, s/n 4200-465 Porto, Portugal

Abstract

The growing use of composite materials in engineering applications has accelerated the demand for computational methods, like multiscale modeling, to accurately predict their behavior. While combining different materials helps achieve optimal structural performance, the complexity of resulting material behavior poses challenges. Multiscale methods based on computational homogenization face a computational bottleneck, limiting widespread industrial adoption. A popular approach to address this is using surrogate models, which have been used to successfully predict a wide range of constitutive behaviors. However, applications involving microscale damage and fracture remain largely unexplored.
This work aims to extend a recent surrogate model using Physically Recurrent Neural Networks(1), to include the effect of debonding at the fiber-matrix interface while capturing path-dependent behavior. In that model, the core idea is to implement the exact material models from the micromodel into one of the layers of the network. Cohesive integration points with a Cohesive Zone Model are integrated within the network, along with the bulk integration points associated to the fibers and/or matrix. The limitations of the existing architecture are discussed and taken into account for the proposal of novel architectures that better represent the stress homogenization procedure.
In the proposed layout, the history variables of cohesive points act as extra latent features that help determine the local strains of bulk points. Different architectures are evaluated starting with small training datasets. To maximize predictive accuracy and extrapolation capabilities of the network, various configurations of bulk and cohesive points are explored, along with different training dataset types and sizes.

*Speaker

Investigating the distribution equilibrium of reinforcement for the microstructure of Mg matrix composites using image processing method

Ali Ercetin*[1], Fatih Akkoyun[2], and Oguzhan Der[3]

[1]Department of Naval Architecture and Marine Engineering, Maritime Faculty, Bandırma Onyedi Eylul University – Turkey

[2]Department of Mechanical Engineering, Faculty of Engineering, İzmir Democracy University – Turkey

[3]Department of Marine Vehicles Management Engineering, Maritime Faculty, Bandırma Onyedi Eylül University – Turkey

Abstract

The ratio of reinforcements is a dominating factor for producing high qualified composites. Besides, the distribution equilibrium of reinforcement is a dominating parameter for determining the actual attributes of the composites. In this study, a practical and accurate image processing approach is presented for the investigation of the equilibrium distribution for a microstructure of Mg matrix composites with the help of computer vision (CV) technology. The Mg matrix composite is determined as a work material to investigate reinforcements distributions of the microstructure. A scanning electron microscopy (SEM) is used to capture images of the microstructure. Initially, the captured images are manipulated using image processing techniques to extract reinforcements locations. The processed images are converted to charts for acquiring peak values of the vertical and horizontal distribution. Next, the microstructure image is divided into sixteen sub-images. Each image is numbered using reinforcement count and the total area of the reinforcement in pixel on the sub-image. The sub-image outputs are normalized to 1 for generating the distribution map of the reinforcements in the microstructures. The results of the experiments are evaluated by comparing the manual distribution mapping with the CV generated distribution map. The experiment results indicate that the distribution equilibrium of the reinforcement is successfully determined by the image processing software. The accuracy of the CV method is found 97% with respect to the manual investigating procedure. Moreover, CV provides detailed information and examination perspective to investigate the homogeneous distribution of the Mg matrix composites.

*Speaker