J. INOUE LAB.

Fusion of Physical Metallurgy and Data Science

Department of Materials and Environmental Science
Large - Scale Experiment and Advanced - Analysis Platform (LEAP)

Materials Informatics in Physical Metallurgy

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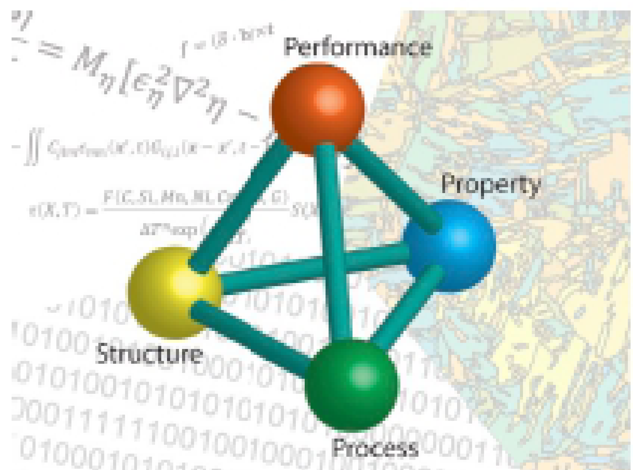
Development of Advanced Structural Materials by combining Physical Metallurgy and Data Science

Enhancement of strength of structural materials meets the requirements in many applications, and especially contributes to the improvement of the resource and energy problem from the body-in-white weight reduction of automobiles. To enhance deformability of structural materials without losing strength, our lab aims to develop new structural materials with enhanced performance by characterizing defects, deformations, and fractures in structural metals and alloys with a help of data-driven material science.

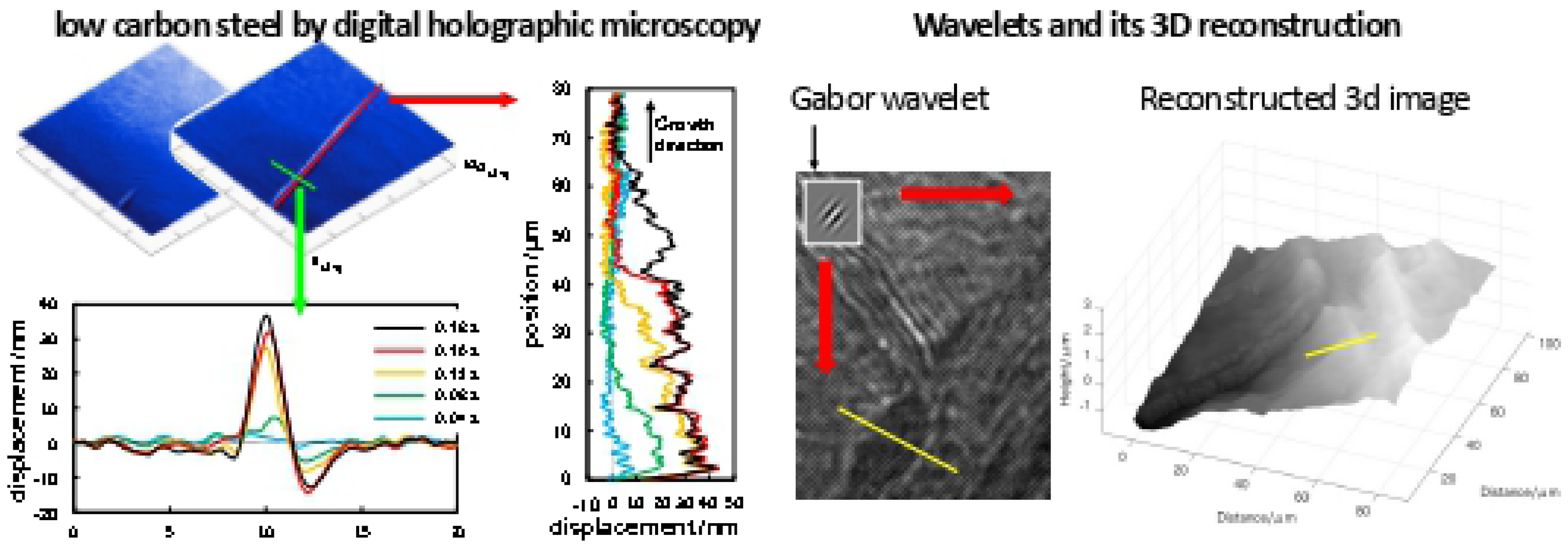


Understanding PSPP relationship from ancestors' wisdom and data

① In-situ observation of local deformation and phase transformation kinetics of metals

In-situ measurement of surface relief induced in low carbon steel by digital holographic microscopy

Hologram convolved with 2D-Gabor Wavelets and its 3D reconstruction



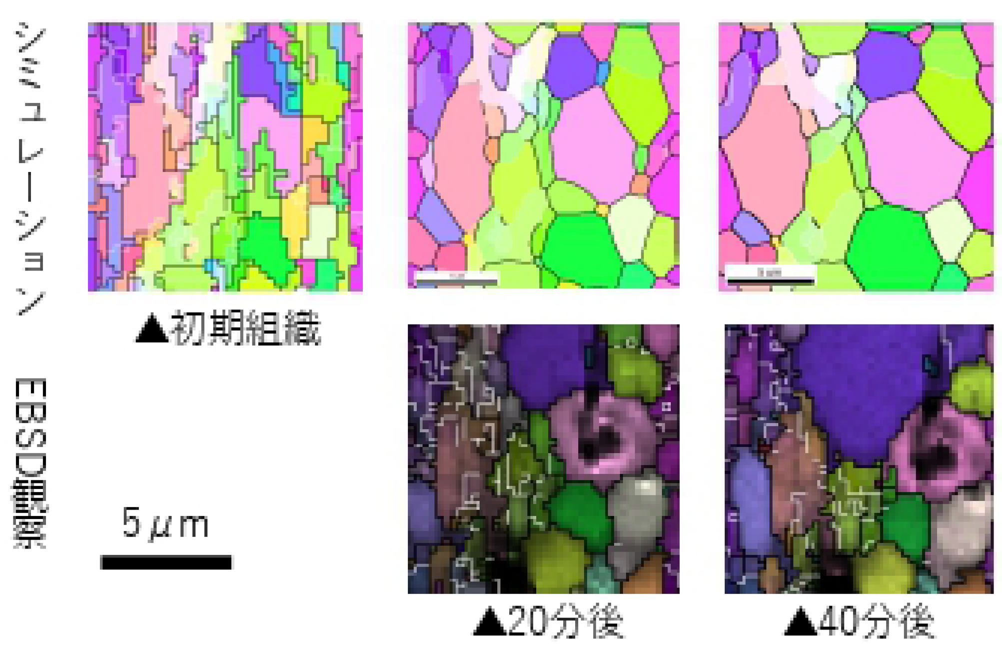
1) S. Komine et al., *Scr. Mater.* 162(2019), 241

C. Lin,et.al., Tetsu-to-Hagane 108 (2022) 360-369

Difference in surface relief effects between bainitic ferrite(left) and Widmanstatten ferrite (right) has been clarified from the in-situ measurement conducted using a newly developed Digital holographic microscope (DHM). The apparatus enables us to measure surface profile of a sample with several nanometer accuracy in real time.

② Estimation of internal properties of Al alloys from EBSD data and phase-field model using data assimilation

Comparison of phase field simulation results and and experimental observations

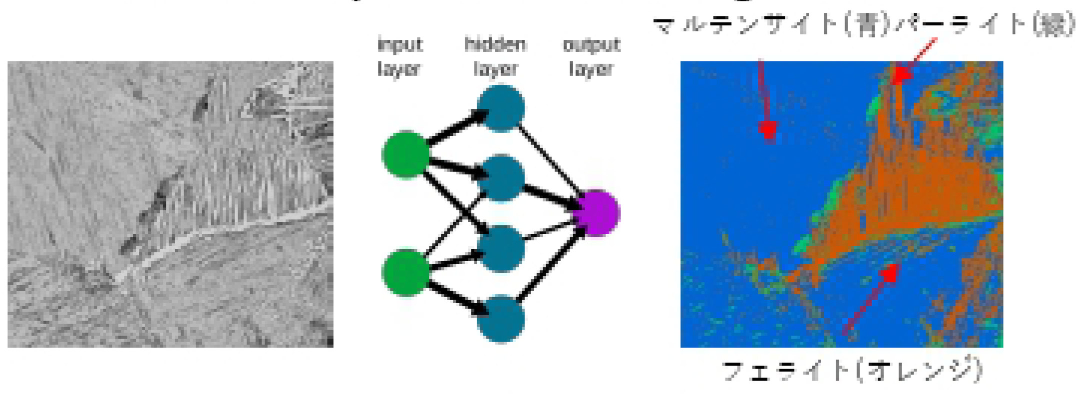


Data assimilation has been applied to clarify the mechanism controlling the recrystallization behavior of industrial pure aluminum. In this example, grain structures are obtained during heat-treatment using EBSD analysis and a phase-field simulation based on subgrain growth model is applied. The precipitation and strain energy stored in each grains are estimated.

③ Unsupervised machine learning applied for the characterization of steel microstructures

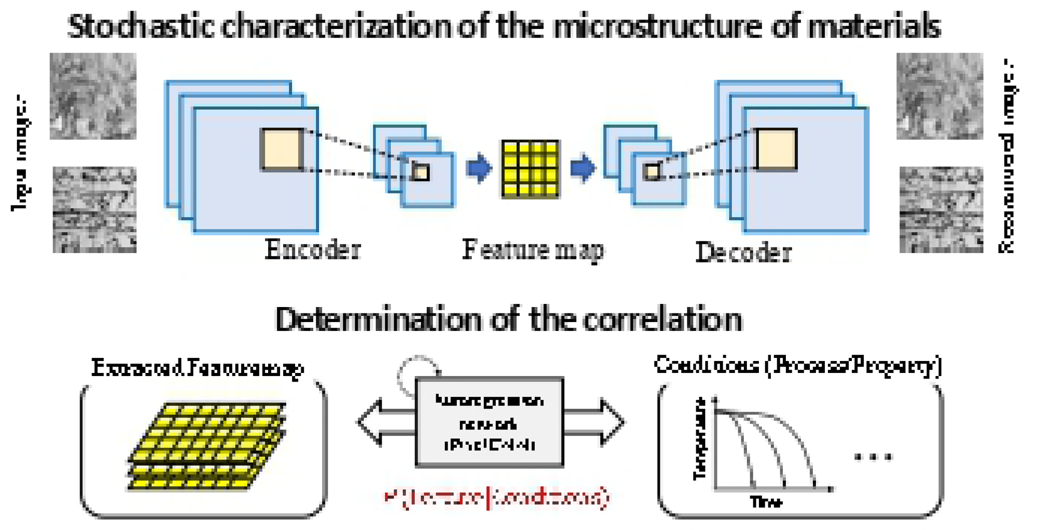
Unsupervised machine learning models are applied to characterize the constituent microstructures of steels, such as ferrite side plate, bainite, and martensite, from optical micrographs. It has been demonstrated that efficient characterization can be performed by the combination of CNN and other machine learning algorithms.

CNN based unsupervised microstructure segmentation



3) H. Kim et al., *Sci. Rep* . 10(2020), 17835.

Stochastic characterization of the microstructure of materials

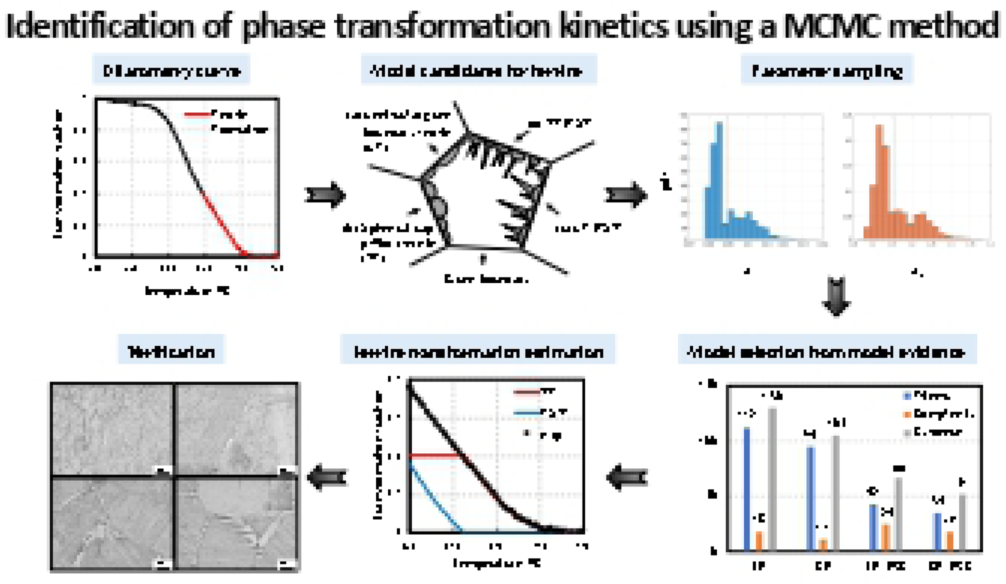


S. Noguchi, H. Wang, J. Inoue, Scientific Reports, 12 (2022) 14238

④ Identification of phase transformation kinetics using sparse modeling

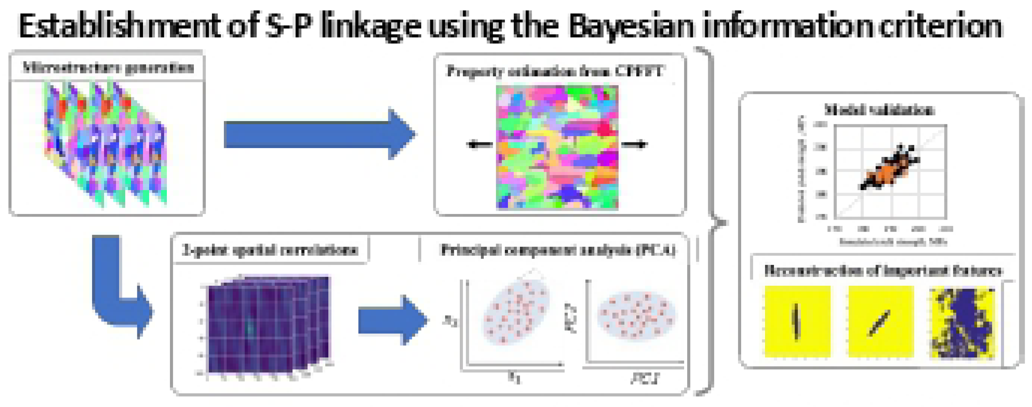
A Bayesian approach has been applied for clarifying the best kinetic model explaining transformation kinetics and mechanical properties of low-carbon steels under different continuous cooling conditions only from experimental and simulation data. It is shown that the method clarifies the underlining physics efficiently without intensive metallographic observations.

Identification of phase transformation kinetics using a MCMC method



5) H. Kim et al., Comp. Mater. Sci. 184(2020) 109837.

Establishment of S-P linkage using the Bayesian information criterion



6) H. Kim et al., *Acta Mater.*, 176(2019), 264