【Grant-in-Aid for Scientific Research (S)】

Quantitative analysis of solidification phenomena using unstructured data obtained by time-resolved tomography

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Project Information	Project Number : 22H04963 Keywords : Solidification/Crystal growth, X-ray imaging, Time-resolved *in-situ* observation, Three-dimensional observation	Project Period (FY) : 2022-2026

Purpose and Background of the Research

● Outline of the Research

This project involves the use of a hard monochromatized X-ray in SPring-8 to observe 2D/3D time-evolution of solidification structures. The observation technique will be developed to combine time-resolved tomography (4D-CT) to follow the solid-liquid interface and X-ray diffraction (XRD) to identify the crystal structure and measure crystal orientation distribution. In addition, reconstruction methods using a phase field model (PFM) will be developed. The developments enable the recording of 3D solidification structures as they are (referred to as “unstructured data”). The formation of solidification structures and casting defects in Al, Mg, Ni and Fe alloys, and the semisolid deformation can be elucidated based on the analysis of the unstructured data. This project will share the unstructured data with the research community.

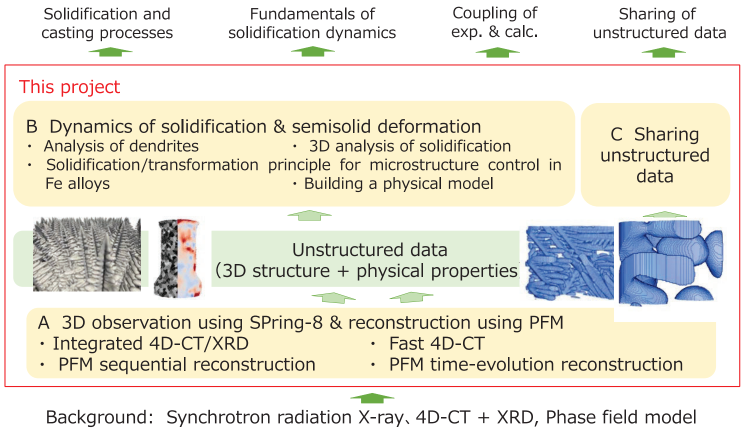

Fig1 Overview of this project

● X-ray imaging for solidification phenomena

Since most metallic materials are produced through solidification processes, it has been of interest to understand how the solidification structure and the defects are formed. However, until recently it has been difficult to verify the phenomena at high temperatures directly. We believe confirming the solidification events by empirical approaches contributes to further understanding and development. Our group has previously developed X-ray imaging techniques (2D and 3D). The novel methods that are developed in the present work, combining 4D-CT/XRD and reconstruction using PFM, will provide new insights.

● Unstructured data

The observation method using 4D-CT/XRD and FPM records the time-evolution of solidification structure non-invasively and allows a true-representation of solidification events without disrupting the processes involved. Solidification phenomena such as fragmentation of dendrite arms, the relationship between microstructure and crystallographic orientation, volume/lattice-constants as a function of temperature, volume change due to phase transformation, and area/curvature of the solid-liquid interface are evaluated by analyzing the unstructured data. Thus, the recorded data is defined as “unstructured data”. The data are expected to be shared with other researchers.

Expected Research Achievements

● Development of 3D observation technique

Fig 2 shows a schematic illustration of the observation technique used in this project. By combining PFM with 4D-CT, quantitative data on dendritic solidification in Al, Mg, Ti, Ni, and Fe alloys will be obtained. Two different reconstruction methods will be developed. One is that the solid-liquid interface is modified by introducing a thermodynamic driving force in PFM. The other is that PFM reproduces the time evolution of dendrites. In the calculation, some physical properties are adjusted. Namely, the procedure is a sort of data assimilation, and the physical properties are also determined.

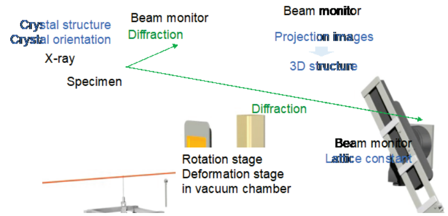

Fig2 Apparatus of 4D-CT/XRD

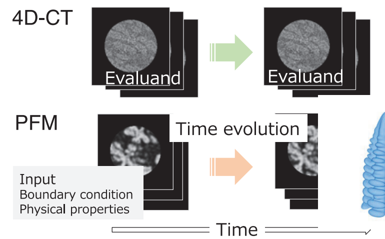

Fig3 Reconstruction using FPM

● Solidification/transformation dynamics

Although it is well known that a dendritic structure evolves during solidification in metallic materials, it is still challenging to evaluate the solid-liquid interface and curvature, which are helpful for understanding solidification structures and defects. In addition, the observed solidification/transformation in Fe alloys differs entirely from the commonly accepted solidification /transformation mechanisms. This project will (1) obtain quantitative data on dendrite growth in Al, Mg and other alloys and (2) understand solidification/transformation in Fe alloys and develop new principles for solidification structure control.

● Micro/macro-dynamics of semisolid

The semisolid state exhibits unique mechanical properties closely related to the formation of casting defects. In our previous work, locally, an interaction between solid grains contributed to non-uniform deformation. In this project, the deformation of a semisolid metal containing more than 10000 solid grains will be observed by 4D-CT. A physical model for the semisolid deformation is to be built based on the observations.

● Sharing of 3D unstructured data

The unstructured data obtained by 4D-CT/XRD are expected to be used for simulating the mechanical properties of dendrite structure and fluid flow in the mushy region. The data will be shared with other researchers for various applications.

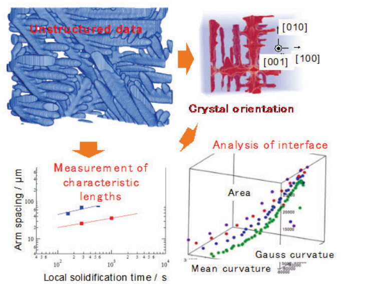

Fig4 Example of analysis using unstructured data

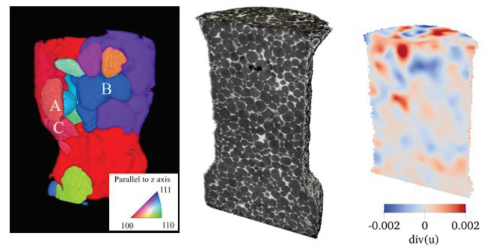

Fig5 Analysis of semisolid deformation. Cristal orientation, solid grains and strain rate.

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