学 位 論 文 内 容 の 要 旨

博士の専攻分野の名称　博士（工学）　氏名　KIM GEUN WOO

学 位 論 文 題 名

Growth Morphology of Solidification Microstructure and Anisotropy of Solid-liquid Interfacial Energy

(凝固組織の成長形態と固液界面エネルギーの異方性)

Growth morphologies of solidification microstructures in metallic materials are largely determined by the anisotropy of solid-liquid interfacial energy. Therefore, the anisotropy of interfacial energy is an essential information in understanding and controlling the solidification microstructures. The interfacial anisotropy in fcc crystals is described by anisotropy parameters ε_1 and ε_2 that characterize $\langle 100 \rangle$ and $\langle 110 \rangle$ growth, respectively. In most of previous studies on dendritic growth in fcc-based metallic alloys, the growth morphology of fcc alloys has been supposed to be $\langle 100 \rangle$ dendrite and, accordingly, only ε_1 has been considered. However, it was recently revealed that the growth morphology of some fcc alloys changes from $\langle 100 \rangle$ to $\langle 110 \rangle$ dendrite by increasing concentration of the solute element, which means that ε_1 and ε_2 depend on the solute concentration. This phenomenon must be taken into account in controlling solidification microstructures with high accuracy. However, details of morphological change and dependence on solidifications conditions and alloy systems have not been clarified yet. Therefore, in this study, morphological diversity of isothermally- and directionally-solidified microstructures associated with different values of ε_1 and ε_2 were closely investigated by means of phase-field simulations.

Meanwhile, the anisotropy parameters of practical alloys have been rarely clarified. To experimentally determine ε_1 and ε_2, an equilibrium shape of the solid must be first realized, and then the solid-liquid interface region should be imaged clearly enough to accurately elucidate a few percent difference of interfacial energy in metallic system. Because of these difficulties, the experimental measurement of anisotropy parameters has been rarely reported. Currently, molecular dynamics (MD) simulation is an effective way of determining ε_1 and ε_2. The capillary fluctuation method and cleaving technique have been developed for computing these anisotropy parameters based on MD simulations and have been successfully applied to several types of materials. However, the accuracy of MD simulations is largely influenced by atomic potential which is not always accurate. Therefore, in this study, a novel method for estimation of anisotropy parameters was proposed by combining phase-field simulations and machine learning overcoming the above-mentioned difficulties.

This thesis consists of six chapters and the organization is described below.

In chapter 1, the importance of anisotropy of solid-liquid interfacial energy was described. In addition, the diversity of the growth morphology and the necessity for measuring anisotropy were explained.

In chapter 2, the quantitative phase-field model which allows for simulations of solidification microstructure with high accuracy was explained.

In chapter 3, the morphological diversity of isothermally-solidified microstructure associated with different anisotropy was investigated by systematically changing ε_1 and ε_2. The growth morphologies were classified into four types, i.e., $\langle 100 \rangle$, $\langle 100 \rangle$−like hyperbranched, $\langle 110 \rangle$−like hyperbranched and $\langle 110 \rangle$ growth. The morphology map for isothermally-solidified microstructure was constructed based on this classification. Furthermore, the dependencies of this map on solidification condition and alloy system were also investigated by changing initial supersaturation and partition coefficient, respectively. It was found that $\langle 100 \rangle$ growth, which is typical growth pattern of fcc-based alloy, hardly occurs when the initial supersaturation is large and/or the partition coefficient is small.

In chapter 4, the morphological diversity of directionally-solidified microstructure associated with the different anisotropy was investigated by systematically changing the anisotropy parameters and the angle between $\langle 100 \rangle$ crystallographic orientation and heat flow direction. The growth morphologies were classified into three types, i.e. $\langle 100 \rangle$, seaweed and $\langle 110 \rangle$ growth. The morphology map for directionally-solidified microstructure was constructed based on the classification. Furthermore, the dependence of the map on solidification conditions such as pulling speed and temperature gradient was investigated. It was found that the seaweed growth region in the space of ε_1 and ε_2 slightly becomes wider as the pulling speed decreases.

In chapter 5, an inverse analysis method of estimating the anisotropy parameters of solid-liquid interfacial energy was developed based on the machine learning. The interfacial shape distribution (ISD) map, which characterizes the details of three-dimensional dendrite morphology, was selected as the input for convolutional neural network, a method of machine learning employed in this study. The feasibility of this approach was tested by performing quantitative phase-field simulations for a free-growing dendrite during isothermal solidification of a model alloy system to obtain training and test data. Both ε_1 and ε_2 were estimated with errors less than 5%, which can be further improved by increasing the size of the training data.

In chapter 6, the overall summary and conclusions of this thesis were presented.