論　文　内　容　の　要　旨

博士論文題目

Development of a new analysis method in two-dimensional reciprocal space map and evaluation of surface atomic arrangement in three-dimensionally nano-fabricated materials using diffraction

（回折法を用いた二次元逆空間マッピングにおける新解析方法の開発、および三次元ナノ加工物質の表面原子配列評価）

氏　　名

竹本　昌平

（論文内容の要旨）

Diffraction methods have been used as useful techniques to determine the atomic structures of materials. In this dissertation the author develops a new diffraction-analysis method in two dimensional (2D) reciprocal space map (RSM) leading to strain distribution of a thin film, and demonstrates surface-sensitive diffraction measurements for usual planar-sample surfaces newly applied to arbitrary-direction oriented surfaces of three dimensional (3D) nano-fabricated materials. These results are described in chapters 2 and 3, respectively.

Chapter 2. So far, crystalline domain size, strain, and strain distribution for poly crystals have been estimated from diffraction peak-position angles and peak-broadening angles by Scherrer method, Williamson-Hall method, and so on. These classical analyses give less accurate results due to the simple estimation. Recently, more accurate analyses were reported; one dimensional (1D) fitting for the shapes of reflection peaks in 2D-RSM shape for poly crystals or thin films, however, 2D fitting, which is important for anisotropic systems, is not established yet.

This chapter presents that the developed 2D-fitting method and results leading to the anisotropic strain distribution, from a few reflections in in-plane 2D RSM of the sample, β-$FeSi_2$(100) nano-film on a Si(001) substrate, measured by in-plane X-ray diffraction (XRD). A main idea is estimation and minimization of the residual between the experimental 2D-RSM reflection shape and model shape, which is induced by the superposition of differently strained domains. This analysis can lead to 2D strain-weight distribution. The strain distribution showed the tendency of a little tensile of *b* axis (i.e., β-$FeSi_2$[010]) and a little compression of *c* axis (i.e., β-$FeSi_2$[001]), mainly +0.1% and -0.3%, respectively, which is consistent with a recent density functional theory calculations.

Chapter 3. Recent highly-integrated Si devices can be achieved with 3D fabrication techniques from constructing on 2D planar surfaces. For instance, fin-type field effect transistors are becoming a promising trend. In such 3D devices, the flatness of side surfaces as the channel region is a key factor to reduce carrier scattering. Thus observations of side surfaces in atomic scale are desired to improve the performance, however, usual scanning or transmission electron microscopies cannot display atomic images of the side surfaces.

This chapter demonstrates the existence of the atomic-ordering reconstruction for atomically-flat side and facet Si surfaces in 3D nano-fabricated structures using reflection high-energy electron diffraction (RHEED): the remarkable application of the diffraction method for usual planar surfaces to other oriented artificial surfaces. In addition, in order to estimate electric conductivity of metal nano-wires on atomically-flat facet surfaces, where the wires are interconnected at facet edges (i.e., 3D wiring electrodes), the author indicated the reduction of the intrinsic conductivity at the facet edges

In summary, the dissertation improves diffraction methods in analysis and application. First the dissertation shows the successful development of a new analysis method which can estimate the strain distribution calculated from the reflection shapes of 2D RSM in in-plane XRD. Second the dissertation shows the creation and observation of atomically-flat and atomically-ordered side and facet Si surfaces of 3D fabricated structures using RHEED at first time. Moreover, the dissertation describes the electric conductivity of the interconnected metals at the facet edge in the atomically-flat facet-surface systems.

氏　名	竹本　昌平

（論文審査結果の要旨）

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As described above, the dissertation improves diffraction methods in analysis and application. Because this knowledge is fundamentally important to the basic science of diffraction field, the committee agreed that this thesis is worth as a PhD thesis for a Doctor of Engineering.