B—1—4 (INVITED) X-Ray Characterization of Single Crystals for Devices with Multiple Crystal Arrangement

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1) Principles and Characterization of Multiple Crystal Arrangement

X-ray diffraction goniometry as well as topography have extensively been employed for characterization of single crystals. In the conventional methods, monochromatization and collimation of the incident beam bundle are made with a slit system, as in the Lang method, where characteristic X-rays such as $MoK\alpha_1$ are used and the spreads in wavelength and angle, $\Delta\lambda/\lambda$ and $\Delta\theta$(rad), are of the order of $10^{-3}\sim10^{-4}$. In order to obtain more detailed or precise information from various kinds of as-grown or processed crystals with various grades of perfection, the control of $\Delta\lambda/\lambda$ and $\Delta\theta$ is made by the multiple crystal arrangement[1], where one or more crystals besides the specimen crystal are used. The multiple crystal arrangement can be classified into two cases. In one case plane crystals of high quality are used[2-5], and in another case is used a bent crystal as monochromator (OMD method[6]). In the former case $\Delta\lambda/\lambda$ is about equal to or less than that of $K\alpha_1$, 5×10^{-4} and $\Delta\theta$ is reduced to less than 10^{-5} rad, while in the latter case the divergent beams with $\Delta\theta\sim10^{-2}$ rad of $K\alpha_1$ are used.

There are several types for the multiple crystal arrangement using plane crystals. In the (+,-) parallel setting, where the lattice spacings of the 1st and 2nd crystals are equal each other, the wavelength dispersion effect is avoided, so that $\Delta\lambda/\lambda$ as large as or larger than 10^{-3} can be utilized to have high intensity. By using asymmetric diffraction for the 1st crystal[1], $\Delta\theta$ can be reduced as small as $10^{-7\sim-8}$ rad[2-4] much smaller than the diffraction range of the specimen crystal, usually 10^{-5} rad. In the (+,+,$\pm$) setting[5], both $\Delta\theta$ and $\Delta\lambda/\lambda$ of the beam incident on the specimen, the 3rd crystal, are made smaller than $10^{-5\sim-6}$, although the decrease of the available intensity can not be avoided, so that any crystal with any lattice spacing can be used as specimen. In the (+,-,+) parallel setting, the 2nd crystal is used as specimen and the 3rd one as analyzer.

2) Applications

Recent studies done in our and some other laboratories will be reviewd[7].

a) Topographic studies.

i) (+,-) parallel setting (plane wave topography): Using quasi-plane wave of X-ray beam($\Delta\theta\sim10^{-6}$ rad), the following studies on dislocation images in Si[8] were made; complete determination of the Burgers vector from the excess number of the equal thickness fringes around a dislocation outcrop; theoretical analysis of the fine structure of the dislocation images observed; sharpening effect of the dis-

location images taken at the off-Bragg condition, corresponding to the weak beam technique in electron microscopy; surface stress relaxation at a dislocation outcrop.

ii) (+,+,±) setting: Observation of imperfections in GGG and $LiNbO_3$ crystals[9].

iii) OMD method: Analysis of warping and wavy structure of B-diffused Si wafers[10], and $GaAs_{0.6}P_{0.4}$ films deposited on GaAs wafers[11].

b) Goniometric studies

i) (+,-) parallel setting: Determination of the distribution functions B or P near the surfaces of Si wafers[12] processed with diffusion; estimation of stacking fault density in Si epitaxial films deposited on sapphire crystals[13].

ii) (+,-,+) parallel setting: Measurements of diffuse scatterings[14] deviated as slightly as $10^{-4\sim-5}$ rad from a normal diffraction peak, for studies on microdefects and slight distortions in Si crystals treated under various conditions such as mechanical polishing, diffusion, and fast neutron irradiation; relative measurement of lattice parameter of Si crystals[15] with resolution of 5×10^{-8}.

iii) (+,+,-) setting: Strain analysis of $LiNbO_3$ crystals diffused with Ti impurities[16].

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