Development of a Simulation Code Combining Takagi-Taupin Equation and Distortion Data by ANSYS

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Introduction

Monochromator crystals irradiated by X-rays from the third generation synchrotron light source are de-formed with heat load. There have been reported thermal deformation analyses of crystals based on the finite element analysis[1,2,3]. However, these reports were limited in the minimization of temperature rise and deformation in crystals, but not the influence of the distortion on the diffraction property. To evaluate the influence, we have developed a simulation code ODDS (Optics for Distorted crystal of Diffraction Simulation) which combines Takagi-Taupin equation[4,5] and distor-tion data calculated by the finite element analysis code ANSYS.

Takagi-Taupin equation

Takagi-Taupin equation is a set of differential equations,

$$\frac{\partial \mathbf{D}_o}{\partial s_o} = -i\pi K C \chi_{-h} \mathbf{D}_h$$

$$\frac{\partial \mathbf{D}_h}{\partial s_h} = -i\pi K C \chi_h \mathbf{D}_o + i2\pi K \beta_h' \mathbf{D}_h$$

$$\beta_h' = -\sqrt{\frac{\mathbf{s}_o \cdot \mathbf{n}}{\mathbf{s}_h \cdot \mathbf{n}}} C|\chi_h| W - \frac{1}{K}\frac{\partial}{\partial s_h}(\mathbf{h} \cdot \mathbf{u}(\mathbf{r}))$$

Here subscripts **o** and **h** represent the incident and dif-fraction wave vectors. **D** is the electric flux densities, $\mathbf{s}_o$ and $\mathbf{s}_h$ the unit vectors of propagating directions, χ_h and χ_{-h} the electric susceptibilities, K the wave number, C the polarization factor, W the normalized angle deviation from the Bragg condition, **h** the scattering vector, **n** the normal vector to the crystal surface and **u**(**r**) the displacement vector located at **r**. The influence of the distortion appears in the second term of the third equation. The distortion data by ANSYS can be substituted to **u**(**r**).

The source file of the ODDS was written by FOR-TRAN. Using HP9000 model 715/33 as CPU, it took 1,800 minutes CPU time and two days on real time to solve the typical model which has 1,000× 5,000 mesh points on fifty different values of W.

ODDS Calculations

In order to check the ODDS, we calculated the diffraction property of a diamond crystal in Laue case on the monochromator of the RIKEN BL[6]. At first the photon flux density from the insertion device was calculated with SPECTRA[7]. The primary parameters for the insertion device were 6keV as the 1st peak energy, 3.7cm as the period length of magnet, 2.8m as the total length and 1.83 as the K value. OEHL[8] was used for the evaluation of the absorbed power at the 100μm thick graphite filter, the 500μm thick beryllium window and 300μm thick diamond. On assumption that the distance between the monochromator and the insertion device was 37m and the slit cut the off-axis light, the total power at the monochromator diamond was 25W. The two dimensional FEM model of diamond holder made of copper was constructed in the ANSYS. A detailed geometry are shown in Fig. 1. Parameters of the boundary conditions were set to 30°C as the cooling water temperature and 5000W/m^{2}K as the heat transfer coefficient at cooling pipe surface.

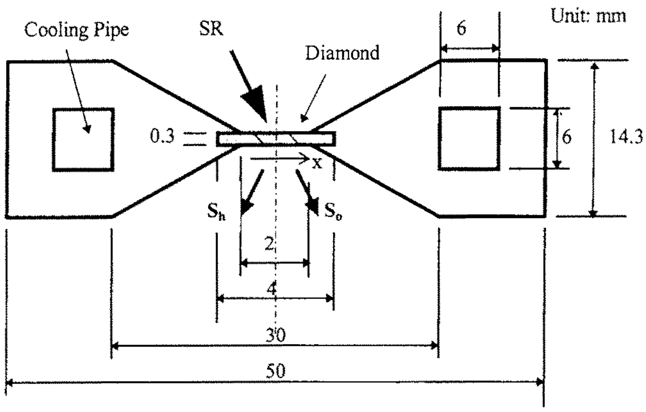

Fig.1 Diamond and diamond holder as a two dimensional model for ANSYS

The results calculated by ANSYS are summarized below. The maximum temperature was 88°C at the irradiated surface and the maximum displacement was 14.2nm at the same point. These values might be over-estimated because the model was not three dimensional but two dimensional. However we could easily know the influence of distortion on the diffraction.

The rocking curves calculated with ODDS are shown in Fig. 2. Because the calculated curves had the Pendellösung fringe, they were smeared out by averaging the several adjacent data in a range of $\Delta W=1.7$ corresponding to the X-ray beam divergence. The peak of the $|\mathbf{D_h}|^2$ rocking curve from the distorted crystal shifted from W=0, which represents a geometrical Bragg condition, to W = 4.3 (9.8 arcsec). It can be explained by the lattice expansion.

In addition, the rocking curve broadening occurs in the distorted crystal. The FWHM of the rocking curve of the distorted crystal was about 2.6 in W scale, while that of the perfect crystal was about 2.2. The change $\delta W=0.4$ (0.91 arcsec) came from the non-uniformity of the reciprocal lattice vector because of the lattice distortion. On the other hand, the slope errors obtained with ANSYS were distributed with an angular width of 0.64 arcsec.

Rocking curve peak shift and width broadening were observed in experiments under high heat load[9].

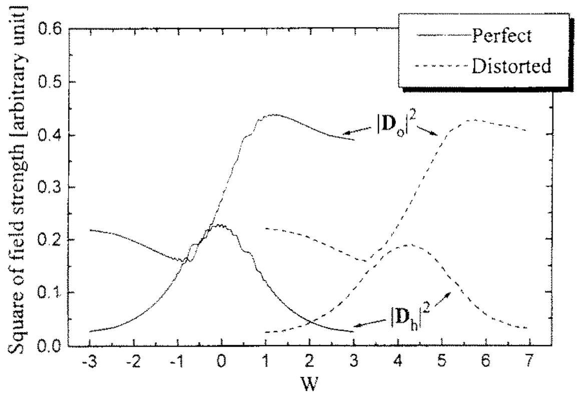

Fig. 2 Rocking curve of perfect and distorted crystals

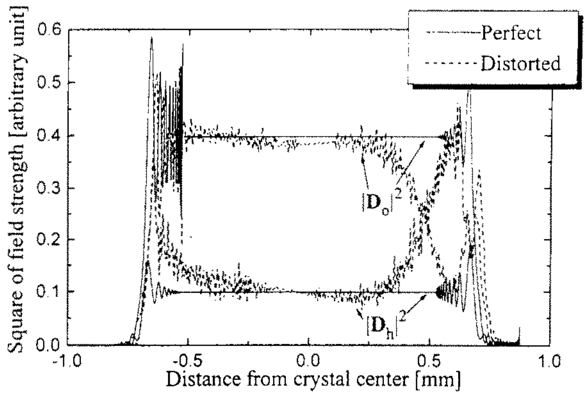

Fig. 3 Field strength of perfect and distorted crystals

The distortion also changes the field distributions. The calculated electric field distributions in the perfect crystal at W=0 and in the distorted crystal at W=4.3 are shown in Fig. 3. The abscissas of Fig. 3 corresponds to the x axis in Fig. 1 and means the surface position where the diffracted and transmitted waves exit. Although not shown in Fig. 3, the distributions in the perfect crystal at any W are constant except at the beam edge. While the distribution in the distorted crystal had remarkable structure and this fringe structures grow large as apart from W=4.3.

Summary

We developed the simulation code ODDS. The peak shift and broadening of rocking curves appeared in the calculated results. These diffraction effects calculated by ODDS were larger than those caused only by the geometrical deformed surface of crystals.

Acknowledgments

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