Development of the tensor CT algorithm for strain tomography using Bragg-edge neutron transmission

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Abstract

The tensor CT algorithm for strain tomography using the Bragg-edge neutron transmission spectroscopy is presented. Crystal lattice strain is not scalar but is a tensor which changes depending on the observation angle. Therefore, since traditional “scalar” CT algorithms cannot be applied to tomography of strain, the development of a “tensor” CT algorithm is needed. Aiming at further developments in the future, we first developed a ML-EM based versatile tensor tomography using of a simple algorithm with small restriction. The basic concept is to simultaneously reconstruct multiple strain-tensor components (scalar quantities of normal strain and shear strain) existing at a certain position. In the actual CT image reconstruction, it is important to consider the angular dependence of each tensor component. Through the simulation studies on axially-symmetric and axially-asymmetric distributions composed of two strain components and experimental demonstration using the axially-symmetric VAMAS standard sample, we found some important points for strain-tensor tomography. The angle-dependent back-projection procedure of ML-EM is indispensable for tomography of each tensor component, but such function also causes an image distortion which can average each strain value along each strain direction. Also, we found that the optimization of the angle-dependent back-projection procedure is important for further improvements of the tensor CT algorithm.

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1. Introduction

Wavelength-resolved transmission imaging using time-of-flight (TOF) spectroscopy of pulsed neutrons can give position-dependent and high wavelength-resolution Bragg-edge transmission spectra of a polycrystalline material. In such an experiment, sharp Bragg-edges can be observed at a neutron wavelength $\lambda = 2d_{hkl}$ (twice of crystal lattice spacing ($d$-spacing) of the plane {hkl}) and the crystal lattice strain information can be deduced quantitatively. As a result, two-dimensional (radiographic) strain imaging over a large area of a bulk specimen can be carried out non-destructively (Santisteban et al. (2002) and Iwase et al. (2012)). Furthermore, the Rietveld-type analysis for the whole spectrum can give radiographic images on crystalline phase (Sato et al. (2013)), texture (preferred orientation) (Sato et al. (2011)) and crystallite size (Sato et al. (2011)).

However, quantitative three-dimensional (tomographic) imaging on such crystallographic information by using computed tomography (CT) has not been achieved yet, although Bragg-edge based CT techniques can become a useful tool for materials science and engineering. Therefore, we considered that development of the Bragg-edge tomography is the next step in terms of the development activity of Bragg-edge neutron transmission imaging.

Tomography of information on strain, crystal orientation and grain/crystallite size is not so easy although it was demonstrated that crystalline phase tomography, without the texture correction, is feasible (Woracek et al. (2014)). This is because strain, orientation and particle size are not scalar values; the observed value depends on the transmission direction of neutrons, namely tensor quantity. Traditional CT algorithms (in this paper, we call “scalar” CT) cannot deal with such “tensor” quantities as they are different from density (absorption-contrast CT) and refractive index (phase-contrast CT). Density and refractive index are scalar quantities independent of the observation angle. As a result, it is impossible to apply the traditional CT image reconstruction algorithms to strain tomography. For this reason, we considered that the development of a new CT, “tensor” CT, is indispensable.

Thus, we are developing a tensor CT algorithm for strain tomography. We are aiming at developing a versatile algorithm for strain tensor because of the following reasons in mind:

- For all objects, not only axially-symmetric strain distributions such as a study by Abbey et al. (2012), but also axially-asymmetric strain distributions have to be reconstructed.
- For more information, all strain components (also shear strain) have to be reconstructed. As a result, finally, the stress imaging using the Bragg-edge neutron transmission spectroscopy will be achieved.
- For the future of neutron imaging society, the algorithm has to be based on simple algorithm with small restriction for the further developments in the future.

For these purposes, we developed a versatile strain tomography that is expanded from a traditional scalar CT algorithm. In this paper, we present the development status of the tensor CT algorithm, some results from simulation calculation studies on axially-symmetric and axially-asymmetric strain tomography, and also results of an experimental demonstration on axially-symmetric strain-tensor tomography using the international standard sample for neutron diffraction strain analysis. Furthermore, some important points and plans for improvement of the tensor CT algorithm are also discussed.

2. Development of the tensor CT algorithm

In this section, we present the basic concept and the data analysis flow of an iterative approximating procedure of the tensor CT image reconstruction algorithm.

2.1. Basic concept

Fig. 1 shows a scheme of the strain $\varepsilon_{\phi \psi}$ observed along a direction $\phi$ and $\psi$ tilted from a certain axes set. The strain $\varepsilon_{\phi \psi}$ is represented by

$$
\varepsilon_{\phi \psi} = \varepsilon_{11} \cos^2 \phi \sin^2 \psi + \varepsilon_{22} \sin^2 \phi \sin^2 \psi + \varepsilon_{33} \cos^2 \psi
+ \varepsilon_{12} \sin 2\phi \sin^2 \psi + \varepsilon_{23} \sin \phi \sin 2\psi + \varepsilon_{31} \cos \phi \sin 2\phi.
$$

(1)
Here, $\varepsilon_{11}$, $\varepsilon_{22}$ and $\varepsilon_{33}$ are normal strains along the axes 1, 2 and 3, respectively. $\varepsilon_{12}$, $\varepsilon_{23}$ and $\varepsilon_{31}$ are shear strains from axis 1 to axis 2, from axis 2 to axis 3 and from axis 3 to axis 1, respectively. These six strain “scalar” components are connected by sine/cosine angular-dependent coefficients as a function of the angles $\phi$ and $\psi$. Thus, the observed value of the strain $\varepsilon_{\psi\varphi}$ at a certain position depends on the observation angle $\phi$ and $\psi$. However, the observed strain $\varepsilon_{\psi\varphi}$ consists of six scalar components. For this reason, we considered that each tensor component, scalar values $\varepsilon_{11}$, $\varepsilon_{22}$, $\varepsilon_{33}$, $\varepsilon_{12}$, $\varepsilon_{23}$ and $\varepsilon_{31}$, has to be reconstructed at each position.

### 2.2. Tensor CT algorithm based on ML-EM

This problem is non-linear one. Therefore, we considered that it is impossible for analytical CT image reconstruction algorithms to solve this problem and that it may be possible by using the iterative approximating CT image reconstruction algorithm. Thus, in this study, we developed a tensor CT image reconstruction algorithm based on the ML-EM (Maximum Likelihood - Expectation Maximization) concept (Dempster et al. (1977)). The first advantage of this algorithm is its simplicity in that is not so special to deal with tensor quantities because the ML-EM algorithm is one of the most useful scalar CT image reconstruction algorithms using the iterative approximation concept.

Eq. (2) shows the equation of iterative approximation from the trial $k$ to the trial $k + 1$, and Fig. 2 shows the parameter definition.

$$
\varepsilon_{ij}^{k+1} = \frac{\varepsilon_{ij}^{k}}{\sum_{d=1}^{D} C_{id} A_{ijd}^{n} \sum_{i=1}^{l} \sum_{j=1}^{l} \varepsilon_{ij}^{k} C_{id} A_{ijd}^{n}} \sum_{d=1}^{D} C_{id} A_{ijd}^{n} \sum_{i=1}^{l} \sum_{j=1}^{l} \varepsilon_{ij}^{k} C_{id} A_{ijd}^{n}
$$

(2)

$\varepsilon$ is a tensor quantity. $i$ indicates a position in a cross-sectional plane of CT image (the total amount is $I$), $j$ means $j$-th scalar quantity of a tensor quantity $e_j$ (the total amount is $J$), $d$ indicates a detector pixel (the total amount is $D$). $C_{id}$ is a geometrical detection probability of the position $i$ by the detector $d$. $A_{ijd}$ is the most important parameter for the tensor CT, a detection probability of $j$-th tensor component of the position $i$ by the detector $d$. $A_{ijd}$ has a function to express the angular dependence of the observed quantity; in other words, this parameter corresponds to the angular-dependent (sine/cosine) coefficients in Eq. (1). $n$ indicates the weight of $A_{ijd}$ for the back-projection procedure in the ML-EM procedure. $p_d$ is the so-called projection data that is the line-integrated value of a physical quantity (crystal lattice plane spacing, in this study) for the neutron transmission path. In the relation between Eqs. (1) and (2), $\varepsilon_{11}$ in Eq. (1) corresponds to $\varepsilon_{11}$ in Eq. (2), $\varepsilon_{22}$ is $\varepsilon_{22}$, $\varepsilon_{33}$ is $\varepsilon_{33}$, $\varepsilon_{12}$ is $\varepsilon_{12}$, $\varepsilon_{23}$ is $\varepsilon_{23}$, and $\varepsilon_{31}$ is $\varepsilon_{31}$, respectively. $\cos^2\phi \sin^2\psi$ in Eq. (1) corresponds to $A_{11id}$ in Eq. (2), $\sin^2\phi \sin^2\psi$ is $A_{22id}$, $\cos^2\psi$ is $A_{33id}$, $\sin^2\phi \sin^2\psi$ is $A_{33id}$, $\sin\phi \sin\psi$ is $A_{33id}$, and $\cos\phi \sin\psi$ is $A_{33id}$, respectively.

The reconstruction procedure of Eq. (2) is explained. The reconstruction flow is almost the same as the scalar ML-EM based CT. Firstly,

$$
\sum_{j=1}^{l} \sum_{i=1}^{l} \varepsilon_{ij}^{k} C_{id} A_{ijd}
$$

(3)

in Eq. (2) is projection data calculated from $\varepsilon$ assumed in the CT image processing. The ratio of measured projection data $p$ to Eq. (3) is derived as follows:
For the back-projection, Eq. (4) is multiplied by $CA^2$. Its summation over all detectors is calculated as follows:

$$\sum_{d=1}^{D} P_d C_{id} A^2_{ijd}.$$  (5)

Eq. (5) is normalized by the normalization factor

$$\sum_{d=1}^{D} C_{id} A^2_{ijd}.$$  (6)

Finally, $\v^j$ is refined to $\v^{i+1}$ by multiplying Eq. (5) divided by Eq. (6), about each $j$-th tensor component at each position $i$. Such procedure is iteratively performed about several to 10 times until a converged CT image is obtained.

The tensor ML-EM CT considers angular dependence of observed quantities, $A_{ijd}$, and the scalar ML-EM CT does not. This is the difference between them. For this reason, the second advantage of this algorithm is its versatility to reconstruct not only axially-symmetric strain distribution, but also axially-asymmetric strain distribution owing to such small restriction. At the same time, this parameter, $A_{ijd}$, is necessary to reconstruct CT images of each tensor component individually.

3. Simulation study on two strain components case of axially-symmetric/asymmetric distributions

In this section, we present simulation calculation results on the tensor CT of axially-symmetric and axially-asymmetric strain composed of two strain components, by using the algorithm presented in the former section. In addition, through this simulation study, we discuss a peculiar issue on the tensor CT algorithm, the determination methodology of the back-projection weight $n$ for $A_{ijd}$.

3.1. Axially-symmetric case like the VAMAS sample

Fig. 3 shows the strain notation at a certain position $(r,\theta)$ on an axially-symmetric strain distribution plane. The axially-symmetric strain distribution means both a strain component along the hoop direction and a strain component along the radial direction. In this case, Eq. (1) is rewritten by

$$\v_{\phi\theta}(r,\theta) = \v_{\theta\theta}(r,\theta)\cos^2\phi(r,\theta) + \v_{rr}(r,\theta)\sin^2\phi(r,\theta).$$  (7)

Here, the three principal axes orient along hoop, radial and axial directions in the cylinder, and the axes 1, 2 and 3 in Fig. 1 correspond to the axes hoop $\theta$, radial $r$ and axial $z$, respectively. In this case, the observed strain $\v_{\phi\theta}$ can be described by only the normal strains $\v_{rr}$ and $\v_{\theta\theta}$. Such strain distribution is observable, for example, in the VAMAS sample (the aluminium shrink-fit ring and plug) which is an international standard sample for

Fig. 3. Notation of strain tensor at the position $(r,\theta)$ in case of axially-symmetric strain distribution such as the VAMAS sample. The green color represents the actually observed quantity, the red color represents its hoop component, and the blue color represents its radial component, respectively.
neutron diffraction strain analysis (cylindrical shape, 5 cm total diameter, 2.5 cm plug diameter and 5 cm height) (Webster (2000)). In the cross-sectional plane, this sample has an axially-symmetric strain distribution of two strain-tensor scalar components.

In this simulation study, the VAMAS sample was assumed. In the CT image reconstruction, it was assumed that the projection data were obtained from 16 directions. The number of ML-EM iteration was 30. Strain images were obtained after the conversion from \( d \)-spacing \( d \) to strain \( \varepsilon = (d-d_0) / d_0 \) because the ML-EM algorithm can accept only values greater than zero but strain can become a value less than zero.

Fig. 4 (a) and (e) show the theoretical strain distributions (simulation phantoms) of (a) hoop strain and (e) radial strain of the VAMAS sample. Fig. 4 (b) and (f) show tensor CT results of no back-projection weight \( n = 0 \) that are equivalent to the scalar CT results. Fig. 4 (c) and (g) show tensor CT results of the back-projection weight of \( n = 1 \), and Fig. 4 (d) and (h) show tensor CT results of the back-projection weight of \( n = 16 \). Firstly, these results indicate that the angular dependent factor \( A_{\phi d} \) with a certain back-projection weight \( n \) is necessary for the CT image reconstruction of each tensor component individually. Additionally, in case of axially-symmetric distribution, as the back-projection weight increases, the hoop strain distribution approaches the true distribution. On the other hand, the radial strain distribution converges to a certain value (in fact, the averaged value) over whole region as the back-projection weight increases, and it does not come close the true distribution even if the back-projection weight decreases. The reason of this phenomenon is discussed in the next section (study on an axially-asymmetric case).

Fig. 4. (a)–(d) hoop strain distributions, and (e)–(h) radial strain distributions of the VAMAS sample, in the simulation. (a) and (e) are theoretical values, (b) and (f) are scalar CT images or tensor CT images of no back-projection weight \( n = 0 \), (c) and (g) are tensor CT images of the back-projection weight \( n = 1 \), and (d) and (h) are tensor CT images of the back-projection weight \( n = 16 \), respectively.

3.2. Axially-asymmetric case

In this section, we present results of a simulation study on an axially-asymmetric case. The three principal axes are oriented along \( x \) (horizontal 1st), \( y \) (horizontal 2nd) and \( z \) (vertical) directions in the Cartesian coordinate, and the axes 1, 2 and 3 in Fig. 1 correspond to the axes \( x \), \( y \) and \( z \), respectively. Eq. (1) is rewritten as

\[
e_{\phi xy}(x, y) = e_{xy}(x, y)\cos^2 \phi + e_{xx}(x, y)\sin^2 \phi.
\]
Actually, in this case, a third strain component (shear strain $\varepsilon_{xy}$) also exists. However, this study aims at establishing the basic algorithm and confirming the versatility of the algorithm, in terms of acceptability of an axially-asymmetric case. Therefore, we limited ourselves to a case of two strain-tensor scalar components.

Fig. 5 shows the simulation results, in the same manner as Fig. 4. The data analysis procedure was the same as the axially-symmetric case (16 angles, 30-times iteration and conversion from $d$-spacing to strain after the reconstruction). The “45°” images in Fig. 5 were obtained by expressing the image along a half angle between the $x$-axis and the $y$-axis.

Firstly, the 45° images were well reconstructed although the images have low spatial resolution. On the other hand, each ($x$ and $y$) strain image is slightly averaged along each ($x$ and $y$) direction although the features of each distribution were detected. Thus, it was found that the axially-asymmetric strain distributions without the shear strain are also reconstructable by the tensor ML-EM CT image reconstruction procedure.

3.3. Discussion of the flat radial strain distribution problem and the angular-dependent back-projection procedure

From the results of the simulation study on the axially-asymmetric case, we found the reason why the radial strain distribution in the axially-symmetric case indicated a flat distribution when $n$ becomes large. In the axially-asymmetric case, the images of each strain component are slightly extended (averaged) along each direction. Such averaging effect is emphasized as the weight $n$ of the angular dependent back-projection increases.
In fact, the $r$ and $\theta$ strain images in the axially-symmetric case are affected by the same phenomenon. However, since the $\theta$ strain image is averaging along the hoop direction, in other words, since the same values exist at the same radius, the hoop strain tomogram of the high weight case like $n = 16$ can indicate the true distribution owing to this averaging effect. On the other hand, the $r$ strain is averaging along the radial direction. As a result, the radial strain tomogram of the high weight case indicates a flat distribution due to this averaging effect. However, the angular-dependent back-projection of a certain weight is indispensable for the tensor CT. Thus, it was found that the optimization of the angular-dependent back-projection procedure is important for the improvement.

4. Experimental demonstration using the VAMAS sample

Finally, we present the first experimental demonstration results of the tensor CT ML-EM algorithm by using the VAMAS sample that has an axially-symmetric strain distribution in the cross-sectional plane.

The pulsed neutron transmission imaging experiment was carried out at BL10 “NOBORU” of MLF at J-PARC in Japan (Maekawa et al. (2009)). The power of the 3 GeV proton accelerator of J-PARC was 300 kW during the experiment. The cold neutron flux at the detector position was about $0.8 \times 10^6$ n/cm$^2$/s. The neutron wavelength resolution at 0.4 nm wavelength was 0.34%. The collimator ratio L/D was 600 owing to the “small” mode of the BL10 rotary collimator.

The neutron TOF-imaging detector used was a $^{10}$B-based GEM (gas electron multiplier) detector developed by Uno et al. (2012) at KEK (High Energy Accelerator Research Organization) in Japan. The pixel size was 800 $\mu$m × 800 $\mu$m. The total detectable area was 9.6 cm × 9.6 cm. The TOF bin width was 10 $\mu$s. The detection efficiency was less than 1% due to the limitation of acceptable counting rate of the DAQ system of the GEM detector. Therefore, a measurement time of about 16 hours for each measurement (with sample and without sample) was necessary. The projection data were obtained in a single direction because this sample has an axially-symmetric strain distribution.

Fig. 6 (a) shows neutron transmission data measured at a certain single pixel. A large Al {111} Bragg-edge due to the texture was observed. Al {111} Bragg-edges of each pixel were analyzed by the single-edge analysis function of the RITS code developed by Sato et al. (2011). The obtained two-dimensional radiographic $d$-spacing map had large errors due to low statistics of the experimental data. For this reason, the averaging was performed along the vertical direction of the cylinder. Additionally, such averaging was performed for the same radius of the cylinder. Finally, the radius-dependent $d$-spacing data were smoothed by the moving average procedure. Fig. 6 (b) shows the $d$-spacing data depending on the distance from the center. Some differences exist between theoretical and experimental data.

![Graphs and images](image_url)

Fig. 6. (a) Bragg-edge transmission spectrum measured at a certain pixel. (b) $d$-spacing of raw analysis data, moving averaged data and theoretical data depending on the distance from the center of the VAMAS cylinder.
The obtained $d$-spacing was from the data averaged along the neutron transmission path. Therefore, we derived line-integrated $d$-spacing values for the transmission thickness. These data were treated as the projection data. The reconstruction procedure was the same as in the simulation study (16 angles, 30-times iteration, and conversion from $d$-spacing to strain after the reconstruction). We made the same 16-angles projection data under the assumption of an axially-symmetric strain distribution. The known information in the reconstruction is only Eq. (7).

Fig. 7 (a) and (b) show the reconstructed cross-sectional images of hoop and radial strains, and (c) shows the comparison result in the absolute value of strain tomogram among experimental, theoretical and simulated data. As well as the simulation studies, the hoop strain was reconstructed with good accuracy and precision, and the radial strain indicated a flat distribution, due to the averaging effect along each strain direction.

![Fig. 7. (a) and (b) cross-sectional images. (c) absolute values with theoretical data and simulated data (the back-projection weight $n = 16)$](image)

5. Conclusion

A new CT image reconstruction method, the tensor CT method, was developed for tomography of the strain tensor dependent on the observing direction. We found the basic concept that each tensor component (scalar value) has to be reconstructed at each position simultaneously. Based on this concept, we developed the ML-EM based tensor CT algorithm that is simple and has small restriction, aiming at further improvements for the future, by expanding a traditional scalar CT algorithm. Through the simulation studies on axially-symmetric/asymmetric strain distributions and the experimental demonstration, we found some points as follows. In the axially-symmetric case, the hoop strain components are reconstructed with good precision and accuracy, but the radial strain ones are averaged along the radial direction. In the axially-asymmetric case, all strain components are reasonably reconstructed although the averaging phenomenon is observed. As a next step, it was found that the optimization of the angular-dependent back-projection procedure of ML-EM is the most important, which causes the averaging phenomenon, but is indispensable for CT of angular-dependent physical quantities. In the future, by further developing this algorithm, we will perform third (shear) and all strain reconstruction, and stress CT, step by step.

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