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EXAFS Analysis and Reinvestigation of the Structure of a Defect-Fluorite-Type Compound, Y_3TaO_7

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The compositional and positional disorder of constituent atoms in Y_3TaO_7 crystals with the defect-fluorite-type structure have been elucidated through analysis of the extended X-ray absorption fine structure (EXAFS) and reinvestigation of the crystal structure with single crystal X-ray diffraction data. EXAFS analysis based on the single shell model gave mean Y–O and Ta–O bond distances of 2.29 and 1.98 Å, respectively. X-ray diffraction study revealed that the structure is essentially of the fluorite type, though Y atoms are displaced along ⟨111⟩ by 0.219(5) Å from the position of Ca in fluorite, and half of the oxygen atoms are also displaced along ⟨001⟩ by 0.54(4) Å from the position of F. The Ta atom is surrounded by at most eight oxygen atoms with Ta–O bond distance of 2.01(2) Å, while the Y atom is surrounded by at most seven oxygen atoms with mean Y–O bond distance of 2.277(7) Å. The mean bond distances and the coordination numbers of metal atoms obtained by X-ray diffraction are generally consistent with those obtained by EXAFS analysis. Most oxygen vacancies in Y_3TaO_7 appear to concentrate around Y atoms. The local structure around Y atoms in Y_3TaO_7 is similar to that in Y_2O_3. Crystal data for Y_3TaO_7 are as follows; cubic, $Fm\bar{3}m$, a = 5.2553(3) Å at 24°C, Z = 1, and D_x = 6.41 g/cm³.

1. INTRODUCTION

R_3TaO_7 compounds, where R denotes rare earth elements, were first reported by Rooksby and White (1). Allpress and Rossell (2) and Shirotinkin *et al.* (3) reported that R_3TaO_7 compounds take different crystal structures according to the size of the R^{3+} cation, varying from a defect-fluorite-type structure for smaller R^{3+} cations to an orthorhombic weberite-type structure for larger R^{3+} cations. Yokogawa *et al.* (4) reported that $xR_2O_3 \cdot (1 - x)Ta_2O_5$ compounds have defect-fluorite-type structures in the range from $x = 0.75$ to $x = 0.80$, where the composition with $x = 0.75$ corresponds to R_3TaO_7.

Ikuma *et al.* (5) measured the oxygen diffusion coefficients of $xY_2O_3 \cdot (1 - x)Ta_2O_5$ (x = 0.75 and 0.8) and Ho_3TaO_7 and suggested that these compounds might be fast ion conductors.

Tanaka *et al.* (6) investigated the structure of Y_3TaO_7 employing the single-crystal X-ray diffraction technique. The analysis was based on a defect-fluorite model, placing metal atoms at Ca positions and oxygens and vacancies at F positions in the fluorite cell. The difference Fourier maps after the final refinement, however, indicated rather large excess and depleted residual electron densities near the atom positions.

In the present study, the extended X-ray absorption fine structure (EXAFS) has been analyzed to obtain detailed information about the local structure of Y_3TaO_7. The EXAFS analysis indicated that the Y–O and Ta–O bond distances are different in the crystal, which cannot occur in the ideal fluorite-type structure. This result led the authors to reanalyze the single-crystal X-ray diffraction data, taking the positional disorder of constituent atoms into account in addition to the compositional disorder. A new structural model of Y_3TaO_7 given in the present paper fits results obtained by both EXAFS and X-ray diffraction.

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2. EXPERIMENTAL

2.1. Preparation of Crystals

The crystals used in the EXAFS analysis were synthesized by the arc-melting method. The starting materials were Y_2O_3 (>99.9% purity, Shin-etsu Chemical Co.) and Ta_2O_5 (99.99% purity, Mitsui Mining Co.). After calcination of the respective chemicals at 1000°C in air for over 10 h, stoichiometric quantities of the oxides were weighed and milled together in an agate mortar with methanol. The mixed powders were pressed into pellets 3 mm in diameter and 4 mm thick. The pellets were melted and rapidly cooled using an arc image furnace (7) to form spherical specimens about 2 mm in diameter.

2.2. EXAFS

A sample of Y_3TaO_7 was measured at the Y*K* and Ta*L*-III absorption edges on the beam line 4C at the Photon Factory of the National Laboratory for High-Energy Physics (KEK) with positron energy 2.5 GeV and a maximum stored current of 350 mA. Crystals of Y_2O_3 and $LiTaO_3$ were used as reference materials. Data were collected in a transmission mode using ion chambers. An exit monochromator with two flat Si (111) crystals was used. The sample was ground and deposited on a tape. The measuring time at each point was 2 sec.

The EXAFS curve, $\chi(k)$, as a function of the wave vector of the photoelectron was obtained from the measured absorption, $\mu(k)$, and the postedge background, $\mu_0(k)$, using an equation

$$\chi(k) = \frac{\mu(k) - \mu_0(k)}{\mu_0(k)}.$$

To remove the underlying background absorption, a linear extrapolation using intensities at two energy points on the preedge was employed. The jump at the absorption edge was normalized by the post- and preedge values of the Victreen coefficients given in the *International Tables for X-Ray Crystallography* (8). The $\mu_0(k)$ curve was approximated by fitting a spline function. The single shell model was assumed for the EXAFS calculation.

2.3. Single-Crystal X-Ray Diffraction

The present study used the three-dimensional X-ray diffraction data collected in the previous study (6). Crystal data are given in Table 1. Experimental conditions are given in Table 2.

After the equivalent reflections were averaged, 83 crystallographically independent reflections with $h \geq k \geq l \geq 0$ were used to refine the structure. Refinements were performed using the full-matrix least-squares program LINKT88 (9), which includes subroutines for extinction corrections after Becker and Coppens (10–12). The atomic scattering factors for Y^{3+} and Ta^{5+} and the values for dispersion corrections were taken from the *International Tables for X-Ray Crystallography* (13). The atomic scattering factors given by Tokonami (14) were used for O^{2-}.

After several cycles of least-squares calculations, it was seen that the type-II extinction correction with a Gaussian mosaic spread (10) gave better agreement between calculated and observed structure factors than the type-I correction. Therefore, further refinements were carried out on the assumption of a type-II correction with a Gaussian mosaic spread.

TABLE 1
Crystal Data for Y_3TaO_7 at 24°C

Space group	*Fm*3*m*
a/Å	5.2553(3)
V/Å^3	145.14(2)
Z	1
D_x/g cm^{-3}	6.41
μ/cm^{-1}	484.6

3. RESULTS

3.1. EXAFS

The $\chi(k)$ curves of Y_2O_3 and Y_3TaO_7 for the Y*K* absorption edge are shown in Fig. 1. The $\chi(k)$ curves of $LiTaO_3$ and Y_3TaO_7 for the Ta*L*III absorption edge are shown in Fig. 2.

The Fourier transforms of the $k\chi(k)$ of the Y*K* edge EXAFS and Ta*L*III edge EXAFS are shown in Figs. 3 and 4, respectively. Limits of the range for the Fourier transform calculation were 3.7–14.5 Å^{-1} for the Y*K* absorption edge and 3.0–13.5 Å^{-1} for the Ta*L*III absorption edge. The Hanning window function was used in the re-

TABLE 2
Experimental Conditions of X-Ray Diffraction

Diameter of specimen/mm	0.088
Radiation	Mo*Kα*
Max. of 2θ/°	120
Monochromator	Graphite
Range of indices	$0 \leq h, k, l \leq 12$
Scan width in 2θ/°	1.8 + 0.5 tan θ
Scan technique	ω-2θ
Scan speed in 2θ/° min^{-1}	2
Maximum number of repetitions for scan	10
Number of reflections measured	546
Number of independent reflections used	83

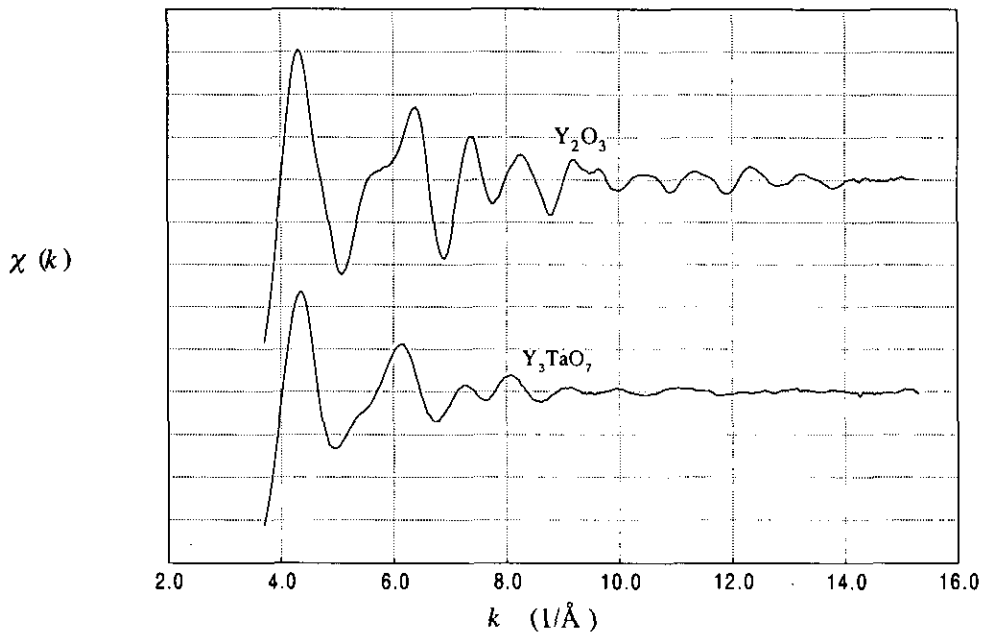

FIG. 1. Normalized EXAFS spectra of Y_2O_3 and Y_3TaO_7 at Y*K* absorption edge.

gion 0.5 $Å^{-1}$ from the limits. Peaks in the region of 1.24–2.39 Å in Fig. 3 and in the region of 1.00–2.11 Å in Fig. 4 were used to determine the bond distances (r) and the coordination numbers (N) and the Debye–Waller factors (σ) around the Y and Ta atoms, respectively. The following phase shift function was adopted,

$$\phi_{ij}(k) = p_0 + p_1k + p_2k^2 + p_3k^{-3},$$

where i and j indicate the absorbing and coordinating atoms, respectively, and p_0, p_1, p_2, and p_3 are the parameters to be refined using a reference material. The value calculated by Teo and Lee (15) was used for the backscattering amplitude.

The mean Y–O bond distance and the coordination number of Y atoms in Y_2O_3 are given by O'Connor and Valentine (16) as 2.28 Å and 6. The mean Ta–O bond distances and the tantalum coordination number in Li TaO_3 were calculated to be 1.985 Å and 6, based on the data reported by Ohgaki *et al.* (17). Using these values,

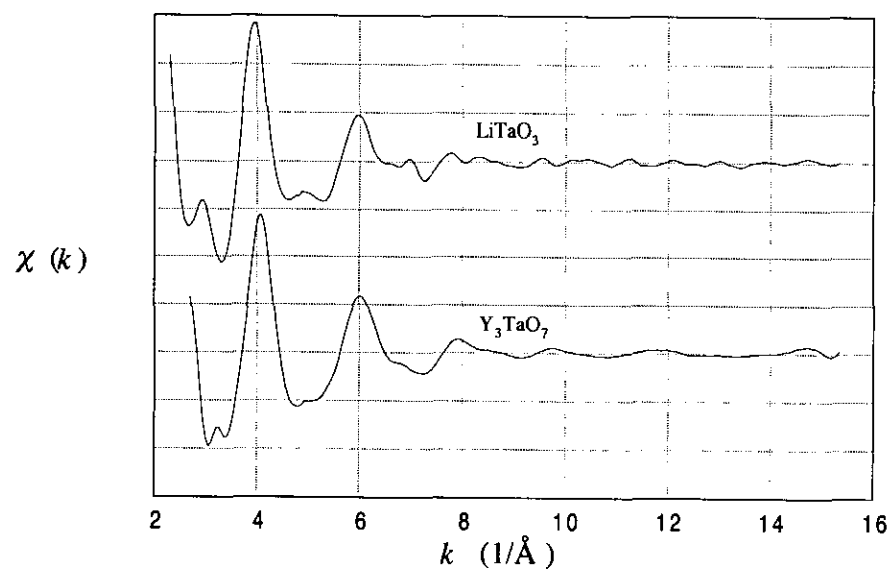

FIG. 2. Normalized EXAFS spectra of $LiTaO_3$ and Y_3TaO_7 at Ta*L*III absorption edge.

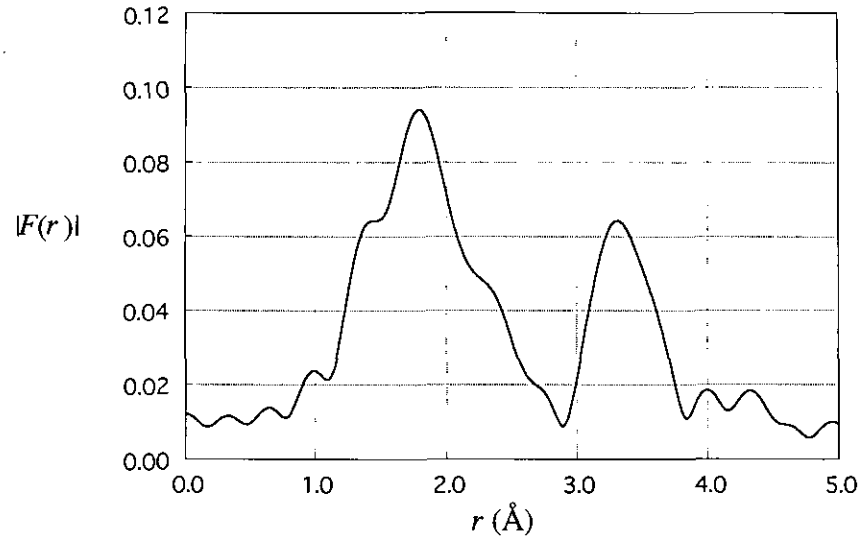

FIG. 3. Fourier transform magnitude of Y*K* EXAFS data of Y_3TaO_7.

the parameters in the phase shift function and the Debye–Waller factors were determined to be $p_0 = 11.843$, $p_1 = -2.522$, $p_2 = 0.09034$, $p_3 = -184.14$, $\sigma = 0.059$ Å^2 for Y–O pairs and $p_0 = 15.0$, $p^1 = -1.0$, $p_2 = p_3 = 0.0$, $\sigma = 0.050$ Å^2 for Ta–O pairs. Mean free path lengths of 7.317 Å for Y_2O_3 and 5.727 Å for $LiTaO_3$, estimated from the reference materials, were assumed in the curve-fitting procedure for Y_3TaO_7. To evaluate the curve-fitting residuals, the following R value was defined:

$$R = \frac{\sum_m |k_m\chi^{\text{obs}}(k_m) - k_m\chi^{\text{calc}}(k_m)|}{\sum_m |k_m\chi^{\text{obs}}(k_m)|}.$$

The R values of Y_3TaO_7 were 0.321 for Y–O pairs and 0.285 for Ta–O pairs, respectively. Results of curve fitting analysis are summarized in Table 3.

3.2. *Single-Crystal X-Ray Diffraction*

(*a*) *Model 1.* First, one of the simplest structural models, referred to as Model 1 hereafter, was examined. In Model 1, all atoms are at the crystallographic sites specified in the fluorite-type structure. This model contains in a unit cell three Y atoms and one Ta atom, which randomly occupy the 4a sites (0, 0, 0 and its symmetry equivalents) of the space group $Fm\bar{3}m$, and seven oxygen atoms and

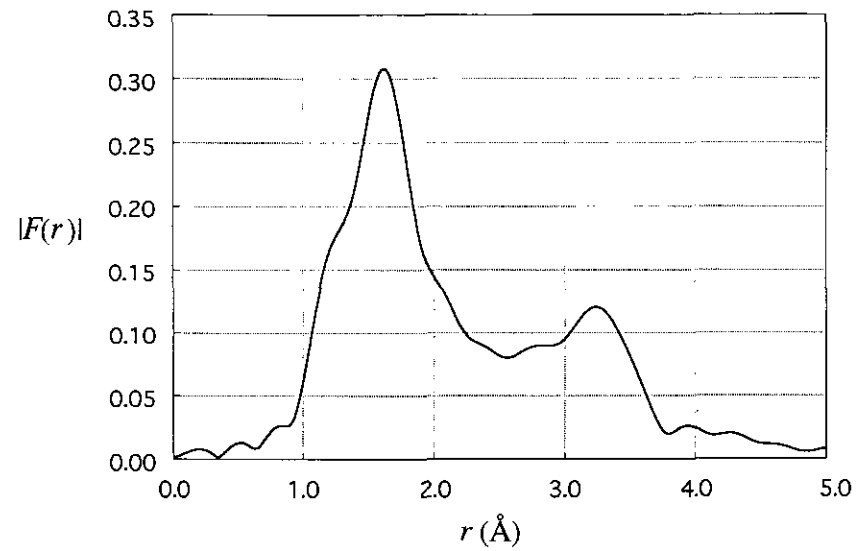

FIG. 4. Fourier transform magnitude of Ta*L*III EXAFS data of Y_3TaO_7.

TABLE 3
Results of Curve Fitting Analysis of EXAFS Spectra of Y_3TaO_7

	r/Å	N	σ/Å^2
Y–O	2.29	5.0	0.079
Ta–O	1.98	8.9	0.06

a vacancy which randomly occupy the 8c sites ($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$ and its symmetry equivalents). This model has already been examined in the previous study (6). It was, however, difficult to compare the results in the previous study with those on the models given in next paragraphs. The main reason was that the refinement in the previous study was carried out using 373 reflection data, which include the crystallographically independent reflections and 11 sets of symmetry-related strong reflections for anisotropic extinction corrections. Therefore, the refinement based on Model 1 was again carried out in the present study. The final R and R_w values employing isotropic thermal parameters and the isotropic extinction correction were 0.0431 and 0.0391, respectively. The isotropic thermal parameters are 0.016(4) Å^2 for Ta and Y atoms and 0.06(1) Å^2 for O atoms. The section of the difference Fourier map through the plane $y = x$ is shown in Fig. 5. Two kinds of positive peaks exist around the origin in Fig. 5; one with the height 4.9 e/Å^3 at the origin, and the other with the height 4.2 e/Å^3 at positions 0.43 Å away from the origin toward the oxygen sites along ⟨111⟩. In addition, peaks with the height 1.0 e/Å^3 exist at positions 0.47 Å away from the oxygen site toward the neighbor oxygen sites along ⟨001⟩. These features observed in the present study are essentially the same as those described in the previous paper, though the heights and shapes of peaks are slightly different.

(*b*) *Model 2.* To explain the residual densities around metal atoms and the discrepancy of bond distances between Ta–O and Y–O revealed by the EXAFS analysis, a positional disorder of metal atoms was taken into account. It is assumed in Model 2 that three Y and 29 vacancies randomly occupy the 32f sites (x, x, x and its symmetry equivalents) of the space group $Fm\bar{3}m$, one Ta and three vacancies randomly occupy the 4a sites (0, 0, 0 and its symmetry equivalents), and seven O and a vacancy randomly occupy the 8c sites ($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$ and its symmetry equivalents) in the unit cell. The final R and R_w values became 0.0261 and 0.0269, respectively. The positional parameter x of the Y atoms was 0.016(4). The isotropic thermal parameters are 0.027(8) Å^2 for Y, 0.010(4) Å^2 for Ta, and 0.058(8) Å^2 for O atoms. The section of difference Fourier map through the plane $y = x$ is shown in Fig. 6. There are positive peaks with height 1.3 e/Å^3 placed 0.36 Å from the Ta atom on the line running along ⟨111⟩ through the Ta atom, and those with the height 1.0 e/Å^3 at positions 0.53 Å from the oxygen atom on the line along ⟨001⟩ through the oxygen atom.

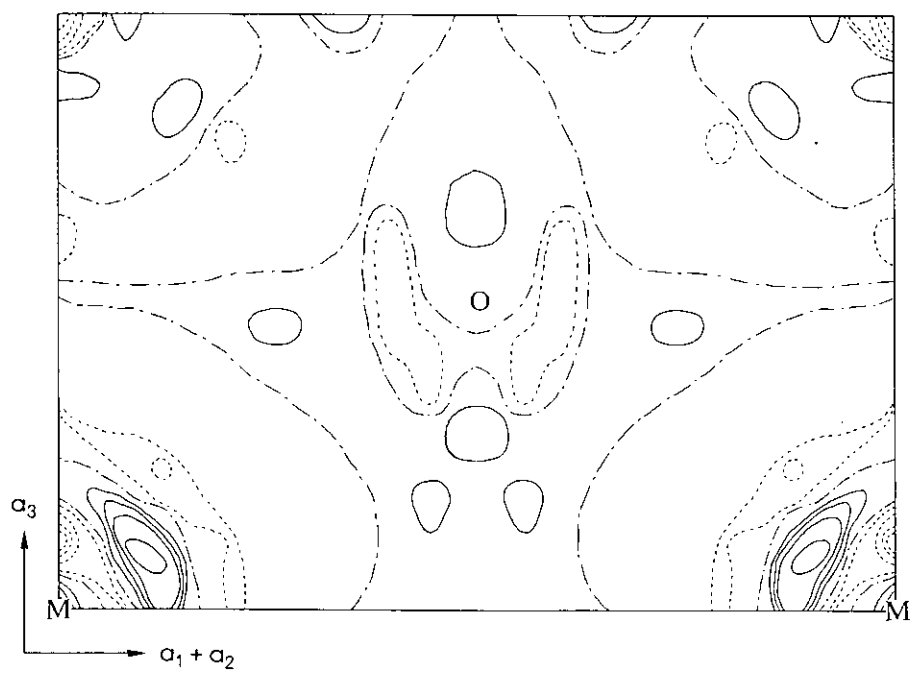

FIG. 5. The section of the difference Fourier map for Y_3TaO_7 through the plane $x = y$ after the refinement based on Model 1. M stands for Ta and Y. Contours are at an interval of 1.0 eÅ^3. Positive, negative, and zero contours are in solid, broken, and dashed–dotted lines, respectively.

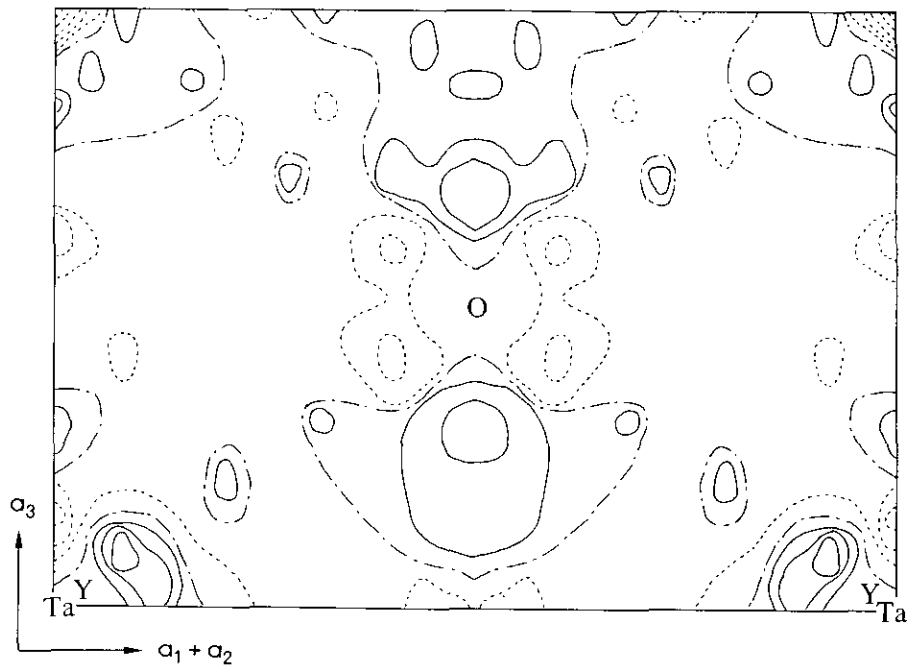

FIG. 6. The section of the difference Fourier map for Y_3TaO_7 through the plane $x = y$ after the refinement based on Model 2. Contours are at an interval of 0.4 $e/Å^3$. Positive, negative, and zero contours are in solid, broken, and dashed-dotted lines, respectively.

A complementary model to Model 2, placing Y at the origin and displacing Ta slightly along ⟨111⟩, gave worse R and R_w values of 0.0281 and 0.0291, respectively. Thus, this model was discarded. Further calculation of Model 2 to examine the possibility of compositional disorder of Ta and Y atoms at 4a and 32f sites was unsuccessful due to strong correlations among the parameters included.

(*c*) *Model 3.* To explain excess residual densities along ⟨001⟩ near the oxygen atoms, a revised model was examined that allowed part of the oxygen atoms to shift slightly along ⟨001⟩, in addition to the displacement of Y atoms along ⟨111⟩ assumed in the Model 2 . In this Model 3, three and one-half oxygen atoms and four and one-half vacancies randomly occupy the 8c sites ($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$ and its symmetry equivalents), referred to as O(1) sites hereafter, and three and one-half oxygen atoms and 44.5 vacancies randomly occupy the 48g sites ($\frac{1}{4}$, $\frac{1}{4}$, z and its symmetry equivalents), referred to as O(2) sites. The final R and R_w values were reduced to 0.0198 and 0.0201, respectively. The structural parameters are given in Table 4. The isotropic extinction parameter was $0.69(2) \times 10^{-4}$ cm. The section of difference Fourier map through the plane $y = x$ is shown in Fig. 7. There are no significant residual peaks. The x parameter of the Y atom slightly increased in comparison with that in the Model 2. In the next stage, the proportion of oxygen atoms to be displaced at O(2) was examined. No significant decrease of the R factor nor any improvement of the residual density maps was observed when the proportion was fixed at values between 0.5 and 0.75. The value less than 0.5 gave worse results. Therefore, the proportion of oxygen at O(2) was fixed at 0.5 in Model 3.

4. DISCUSSION

The Ta–O distance in Y_3TaO_7 obtained by the EXAFS analysis was 1.98 Å, which is approximately 0.30 Å shorter than that of 2.2756(1) Å obtained in Model 1 by assuming a simple fluorite-type structure. On the other hand, the Y–O bond distance obtained by EXAFS analysis was 2.29 Å which is approximately the same as that of 2.2756(1) Å in Model 1. The coordination numbers of Y and Ta atoms determined by the EXAFS analysis are 5.0 and 8.9, respectively. The discrepancy between Model 1 and the EXAFS results can be explained with Model 3.

In Model 3, Ta atoms are located at the Ca sites in the fluorite-type structure, while Y atoms are displaced from these along ⟨111⟩ by 0.219(5) Å. Half of the oxygen atoms

TABLE 4
Structural Parameters of Y_3TaO_7 Based on Model 3

Atoms	Population	x	y	z	$U_{iso}/Å^2$
Y	0.09375	0.0241(9)	0.0241(9)	0.0241(9)	0.016(7)
Ta	0.25	0.0	0.0	0.0	0.010(3)
O(1)	0.43750	0.25	0.25	0.25	0.031(4)
O(2)	0.07292	0.25	0.25	0.353(8)	0.021(5)

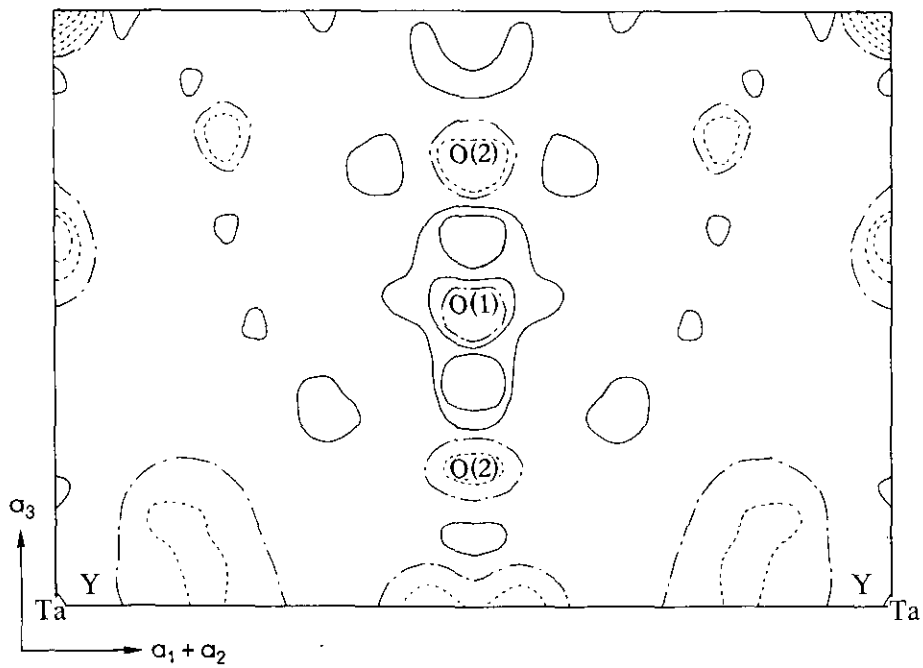

FIG. 7. The section of the difference Fourier map for Y_3TaO_7 through the plane $x = y$ after the refinement based on Model 3. Contours are at an interval of 0.4 $e/Å^3$. Positive, negative, and zero contours are in solid, broken, and dashed–dotted lines, respectively.

are located at the F sites in the fluorite-type structure, while the remaining half are displaced from these along ⟨001⟩ by 0.54(4) Å. The local structure around the metal atom is schematically illustrated in Fig. 8. Surrounding the metal atom near the origin, there are one O(1) site and six O(2) sites in a octant and, therefore, 8 O(1) and 48 O(2) sites in the eight octants. Since the Ta atom is at the origin, there are one O(1) site at 2.2756(1) Å, three O(2) sites at 2.63(3) Å, and three O(2) sites at 2.01(2) Å in a octant. Among these, the bonds of 2.2756(1) and 2.63(3) Å are generally too long for the Ta–O distance if the sum of their ionic radii is taken into account. In addition, the O–O distance of 0.77 Å between three O(2) sites at 2.01(2) Å in a octant is too short to accommodate more than one oxygen in the octant. Therefore, the Ta atom is thought to be surrounded, at a maximum, by eight O(2) atoms in respective octants at a distance of 2.01(2) Å. The Ta–O bond distance of 2.01(2) Å agrees with that of 1.98 Å obtained by the EXAFS analysis within the error. The coordination number of 8 is also consistent with that of 8.9 obtained by the EXAFS analysis, since the latter is estimated to have an error of approximately ±1.

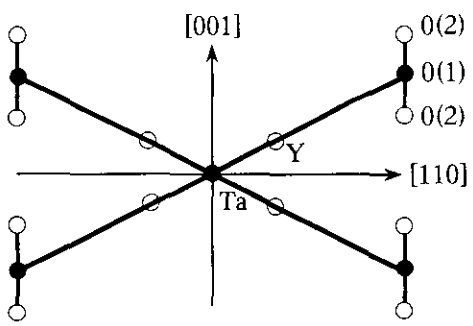

FIG. 8. Structure of Y_3TaO_7 through the plane $x = y$ based on Model 3. Shifts of atoms are exaggerated.

Since the Y atom is displaced slightly from the origin, there are many possible Y–O bond distances. The possible Y–O bonds around the Y atom located at x, x, x with $x = 0.0241(9)$ are listed in Table 5. Removing bonds shorter than 2.2 Å and longer than 2.4 Å from Table 5 leaves nine Y–O bonds. The values of 2.2 and 2.4 Å were adopted as criteria for two reasons. One is that the EXAFS results indicate an average bond distance of 2.29 Å for this crystal. The other is that all Y–O bond distances in the structure of Y_2O_3 fall in the range from 2.243(4) to 2.331(4) Å, as stated later. Among the nine oxygen sites, three are the O(1) sites at a distance of 2.212(5) Å in the octants II, IV, and V, three are the O(1) sites at a distance of 2.358(5) Å in the octants III, VI, and VIII, and three are the O(2) sites at a distance of 2.23(2) Å in the octant VII. The last three O(2) sites in the octant VII are too close with each other to accommodate more than one oxygen. Therefore, the maximum coordination number of the Y atom becomes seven. In other words, seven oxygens in seven octants can surround the Y atom in the remaining octant. The mean distance of 2.277(7) Å for

TABLE 5
Possible Y–O Bonds around the Y Atom Located at x, x, x, with $x = 0.0241$

I(+ + +)			V(+ + −)		
O(2)	1.80(2)	×3	O(2)	1.90(2)	
O(1)	2.056(5)		O(2)	1.98(2)	×2
O(2)	2.41(3)	×3	* O(1)	2.212(5)	
			O(2)	2.54(3)	×2
			O(2)	2.60(3)	
II(− + +)			VI(− + −)		
O(2)	1.90(2)		O(2)	2.07(2)	×2
O(2)	1.98(2)	×2	O(2)	2.14(2)	
* O(1)	2.212(5)		* O(1)	2.358(5)	
O(2)	2.54(3)	×2	O(2)	2.67(3)	
O(2)	2.60(3)		O(2)	2.72(3)	×2
III(− − +)			VII(− − −)		
O(2)	2.07(2)	×2	* O(2)	2.23(2)	×3
O(2)	2.14(2)		O(1)	2.495(5)	
* O(1)	2.358(5)		O(2)	2.84(3)	×3
O(2)	2.67(3)				
O(2)	2.72(3)	×2			
IV(+ − +)			VIII(+ − −)		
O(2)	1.90(2)		O(2)	2.07(2)	×2
O(2)	1.98(2)	×2	O(2)	2.14(2)	
* O(1)	2.212(5)		* O(1)	2.358(5)	
O(2)	2.54(3)	×2	O(2)	2.67(3)	
O(2)	2.60(3)		O(2)	2.72(3)	×2

Note. The octant (+ − +), for example, means $x > 0$, $y < 0$, $z > 0$. Distances marked by * are considered as the most plausible Y–O bonds.

these seven Y–O bonds agrees well with the 2.29 Å obtained by EXAFS.

In the above discussion, oxygen vacancies are not necessarily taken into consideration. The chemical composition of Y_3TaO_7 can be written as $4[(Y_{3/4},Ta_{1/4})O_{2-\delta}]$ with the amount of oxygen vacancy $\delta = 0.25$ in terms of the defect-fluorite-type composition. If all oxygen vacancies were assumed to concentrate around Y atoms, the mean coordination number of Y atoms becomes 6.7. As shown in 3.1, the EXAFS analysis gave a coordination number of 5, which is also smaller than the value of 7 derived in the former paragraph. Therefore, it is plausible that most oxygen vacancies concentrate around Y atoms in the crystal, yielding a mean coordination number of nearly 6.7 for Y atoms.

Crystals of Y_2O_3 have the C-type structure (16, 18) with space group $Ia3$. The unit cell has a doubled **a** length in comparison with the fluorite cell, containing eight Y(1) atoms and 24 Y(2) atoms with the coordination number of 6. Oxygens around Y(1) occupy six corners of a cube at 2.284(3) Å. The missing two corners are related by the body diagonal of the cube, which provides an octahedral shape for the coordination polyhedra of $Y(1)O_6$. Oxygens around Y(2) also occupy six corners of a cube, but the two missing corners are located at one of the face-diagonals of a cube, resulting a deformed octahedral shape for $Y(2)O_6$. Bond distances of Y(2)-O are 2.243(4) Å (×2), 2.274(4) Å (×2) and 2.331(4) Å (×2). It is noted that the Y–O bonds in Y_2O_3 crystal are roughly grouped into two with different lengths centred at 2.267(4) and 2.331(4) Å. This is comparable with the result that the Y–O bonds in Y_3TaO_7 crystal are also grouped into two groups with lengths centered at 2.217(9) Å (three 2.212(5) Å plus one 2.23(2) Å) and 2.358(5) Å (three 2.358(5) Å). Therefore, a close similarity can be pointed out between the local structure around the Y atoms in Y_2O_3 and Y_3TaO_7. Actually, if one of three oxygens at a distance of 2.358(5) Å in the octants III, VI, or VIII is missed in Y_3TaO_7, the resultant YO_6 polyhedron becomes quite similar in shape to $Y(2)O_6$ in Y_2O_3.

5. CONCLUSION

The EXAFS analysis on Y_3TaO_7 crystals prepared by the arc-image technique revealed that the mean Y–O and Ta–O bond distances are 2.29 Å and 1.98 Å, respectively, and the coordination numbers of Y and Ta atoms are 5.0 and 8.9, respectively.

Single-crystal X-ray diffraction study on the crystal revealed that the structure is essentially of the fluorite type one though the Y atoms are displaced along ⟨111⟩ by 0.219(5) Å and half of the oxygen atoms are also displaced along ⟨001⟩ by 0.54(4) Å. The final R and R_w values were 0.0198 and 0.0201, respectively, for the 83 observed reflections. The Ta atom is surrounded by at most eight oxygens, with Ta–O bond distance of 2.01(2) Å. The Y atom is surrounded by at most seven oxygens, that is, three at 2.212(5) Å, three at 2.358(5) Å, and one at 2.23(2) Å. The mean Ta–O and Y–O bond distances are 2.01(2) and 2.277(7) Å, respectively, which agrees well with the EXAFS results within error. Most of the oxygen vacancies are supposed to concentrate around the Y atoms in Y_3TaO_7.

The local structure around the Y atoms in Y_3TaO_7 is similar to that in Y_2O_3 in two points: (1) both compounds have smaller coordination number than that of 8 in fluorite, and (2) the Y–O bonds are grouped into two groups with different bond lengths.

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