Crystal structure of Er^{3+}-α-SiAlON

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1. Introduction

SiAlON ceramics are Si_3N_4 based ceramics and are mostly known for high-temperature and high-endurance applications due to their ability to withstand high structural load and their excellent chemical and thermal stability. Taking an advantage from their superior mechanical, thermal and chemical stabilities, these materials have also been investigated recently for the possibility of functional applications such as downconversion phosphor materials for solid-state lighting. In spite of the huge number of experimental investigation of α-SiAlON ceramics, the structure of Ln^{3+} doped α-SiAlON are complex and not precisely determined, because the random distribution of O and N leads to fluctuating bond length.

Cole et al., J. Mater. Sci. 1991, used the technique of extended X-ray absorption fine structure (EXAFS) spectroscopy in Er-doped α-SiAlON to investigate the local environment surrounding the Er^{3+} stabilizing cation. The work confirms the seven-fold coordination of the modifying cation within the interstices, but indicates a N:O ratio of 5:2 rather than the 6:1 ratio as indicated by the Rietveld refinements of Izumi et al, J. Mater. Sci. 1984.

In this project we performed a combined experimental and first principle calculation to determine an accurate crystal structure of Er3+ doped α-SiAlON. We performed neutron diffraction experiment to determine precisely the coordination environment of Er^{3+} in the lattice and validate the result of our first principle calculation of electronic structure of Er^{3+}-α-SiAlON.

2. Experiment

The powder neutron diffraction experiment was carried out at Japan Proton Accelerator Research Complex (J-PARC), Japan, using Super High Resolution Powder Diffractometer (SuperHRPD) backward detector. The measurement was done at room temperature for 24 hours. The obtained diffraction data was used for the Rietveld refinement using Z-Rietveld software.

3. Results

The Rietveld data fit on the neutron diffraction data of the hot-press-sintered Er^{3+}-α-SiAlON ceramic and the difference pattern between simulated and the experimental data are shown in Figure 1. α-SiAlON is the most dominant phase observed. Small amount of impurity phases are also observed. The impurity phases originate from small traces of ß-SiAlON. The structural details of the Er^{3+}-α-SiAlON ceramic as calculated by Rietveld refinement is shown in Table 1. Taking into account the difference in composition between our sample and by Cao et al. (J. Mater. Sci. 1993), for the neutron diffraction, there is a good agreement in the lattice parameters and atomic positions.

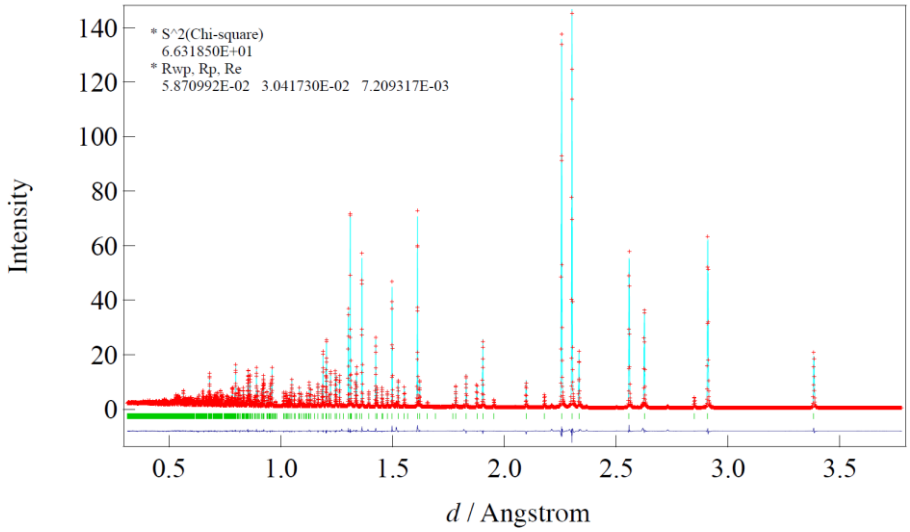

Figure 1. Rietveld refinement result of the neutron diffraction pattern of Er^{3+}-α-SiAlON.

Table 1. Refined structural parameters of Er^{3+}-α-SiAlON in space group P31c (No.159).

Space group	Lattice constants	a	b	c	alpha	beta	gamma
159_1		7.8145420(6)	7.8145420(6)	5.6988144(10)	90	90	120

Atom	Symbol	Occupancy	x	y	z	B Iso
1	Er	0.1615376442	0.3333333333	0.6666666667	0.2480(3)	1.326(19)
2	Si	0.8187002515	0.50942(3)	0.08173(3)	0.21198(3)	0.593(3)
3	Al	0.1812997485	0.50942(3)	0.08173(3)	0.21198(3)	0.593(3)
4	Si	0.9186017729	0.16870(2)	0.25177(2)	0.00188(4)	0.444(2)
5	Al	0.0813982271	0.16870(2)	0.25177(2)	0.00188(4)	0.444(2)
6	N	0.8150219423	0	0	-0.00007(4)	0.4426(18)
7	O	0.1849780577	0	0	-0.00007(4)	0.4426(18)
8	N	0.7198948215	0.3333333333	0.6666666667	0.64958(3)	0.755(3)
9	O	0.2801051785	0.3333333333	0.6666666667	0.64958(3)	0.755(3)
10	N	0.8345229833	0.343084(11)	-0.047933(10)	-0.016172(19)	0.5763(11)
11	O	0.1654770167	0.343084(11)	-0.047933(10)	-0.016172(19)	0.5763(11)
12	N	0.8253400857	0.318718(12)	0.317243(13)	0.24737(2)	0.5799(11)
13	O	0.1746599143	0.318718(12)	0.317243(13)	0.24737(2)	0.5799(11)

4. Conclusion

Powder neutron diffraction experiment of hot-press-sintered Er^{3+}-α-SiAlON was successfully accomplished. Obtained data was analyzed using the Rietveld refinement technique. The sintered ceramic contains dominant α-SiAlON phase with a trace amount of impurity phases. Identification of the other impurity phases present in the material and the determination of coordination environment of Er^{3+} in the lattice of α-SiAlON are under way.