Local structure of Lu doped in high creep resistant Al_2O_3

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Introduction

Addition of small amount of a third element into Al_2O_3 ceramic have been extensively studied to improve mechanical properties especially at high temperature. Recent years, Yoshida et al. have found that Lu doping is particularly effective in improving the high-temperature creep resistance of poly crystalline Al_2O_3[1]. TEM observation shows that doped Lu atoms condensed in the grain boundary of Al_2O_3[1]. Local environment around Lu atoms at grain boundary is directly connected to the mechanical properties of Lu-doped Al_2O_3. However, the role of the Lu has not been well understood. In this present work, we study the local structure around Lu atoms obtained by EXAFS.

Experimental

Mixture of high-purity Al_2O_3 and Lu acetate pressed into bars with cemented carbide under a pressure of 33MPa, and isostatically-pressed under a pressure of 100MPa. The pressed mixture was sintered at 1400°C for 2 hour in air. The amount of doped Lu was 0.05at%. Lu L_{III}-edge XAFS spectra were measured using fluorescence mode at the BL12C station with double Si(111) monochromator at 20K. In the curve fitting analysis, parameters of the phase shift, the back scattering amplitude and the electron mean free path were obtained using FEFF program.

Results and discussion

Fig. 1 shows (a) k^3Lu L_{III}-edge EXAFS, $k^3 \cdot \chi(k)$, of 0.05at%Lu-Al_2O_3 and Lu_2O_3 as reference sample and (b) Fourier transform of them. F(r) of Lu in Al_2O_3 exhibit only one peak at 1.9Å, which corresponds to the first nearest Lu-O pair, while Lu_2O_3 shows long distance correlations. Such vanishing of the long distance correlation of F(r) of Lu in Al_2O_3 suggests strong distortion of the local structure around Lu atoms. The results of the curve fitting analysis of the Lu-O correlation of Lu in Al_2O_3 are listed in a table 1. Since, one Gaussian fitting did not converge well in this curve fitting procedure, we use double Gaussian fitting for the Lu-O peak of Lu in Al_2O_3. Mean cation-oxygen distance in the octahedral site (coordination number is six) of the Lu_2O_3 is 2.24Å and that of the Al_2O_3 is 1.91Å. Consequently, it can be concluded that doped Lu in Al_2O_3 mainly occupy the octahedral site which similar to that in the Lu_2O_3. Larger mean coordination number of 6.5, however, suggests that Lu atoms also occupy the site with large volume. This heterogeneity of the local structure around Lu atoms causes large Debye-Waller factor. The local structure around Lu obtained from EXAFS reflects the condensation of Lu in the grain boundary of Al_2O_3.

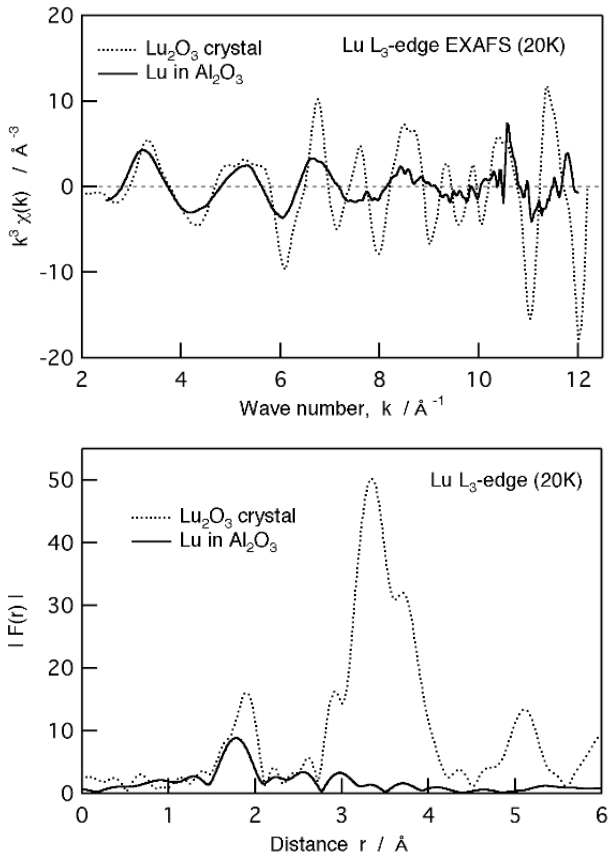

Fig.1 (a) k^3 Lu L_{III}-edge EXAFS, $k^3 \cdot \chi(k)$, of 0.05at%Lu-Al_2O_3 and Lu_2O_3 and (b) Fourier transform of them.

Table 1: Curve fitting results for Lu-O correlation of Lu L_{III}-edge EXAFS for Lu in Al_2O_3. N, R and σ correspond to coordination number, atomic distance and Dwbye-waller factor, respectively.

	N	R(Å)	σ(Å)
Lu_1-O	1.3	2.02	0.06
Lu_2-O	5.2	2.34	0.11

References

[1] H. Yoshida et al., Int. J. Inorg Mater. **1**, 229 (1999)

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