Local structure of solid and molten strontium dichloride

Yoshihiro OKAMOTO[1*], Tsuyoshi YAITA[1], Haruhiko MOTOHASHI[2], Katsumi KOBAYASHI[3], Noriko USAMI[3]

[1]Japan Atomic Energy Research Institute, Tokai-mura, Naka-gun, Ibaraki 319-1195, Japan
[2]SPring-8 Service Corporation, Kouto, Mikazuki-cho, Hyogo, 678-1205, Japan
[3]KEK-PF, Tsukuba, Ibaraki 305-0801, Japan

Introduction

We have studied the local structure of molten salt systems by high temperature XAFS technique[1]. In the present study, we report the local structure of solid and molten $SrCl_2$.

Experimental

The XAFS measurements of solid and molten $SrCl_2$ (Sr K-dege) were performed in transmission method at the BL27B station in the KEK-PF. The samples were sealed off in the quartz cell under reduced pressure(<10^{-5}Torr). Details of the XAFS measurement of molten salts are described in ref.[2]. The XAFS spectra were obtained at room temperature, 1073 and 1273K. The XAFS data was analyzed by using WinXAS code[3].

Results and discussions

The Fourier transform magnitude |FT| functions for solid and molten $SrCl_2$ are shown in Fig.1. Structural parameters of the nearest Sr^{2+}-Cl^- correlation determined from the curve fitting are listed in Table 1. The averaged distance does not change by melting. On the other hand, the coordination number decreases from 8 to 6.6. It corresponds to the volume change $\Delta V_m/V=0.13$ at melting. At 1073K, it can be considered that the sample is in a superionic state because of increasing in Debye-Waller factor and unchanged coordination number.

The molecular dynamics calculation of solid and molten $SrCl_2$ was performed by using pair potentials proposed by Gillan and Dixon[4]. The XAFS function $k^3\chi(k)$ was synthesized by using the GNXAS[5] from the MD results. The XAFS functions at 1073 and 1273K were successfully reproduced by the MD simulation as shown in Fig.2.

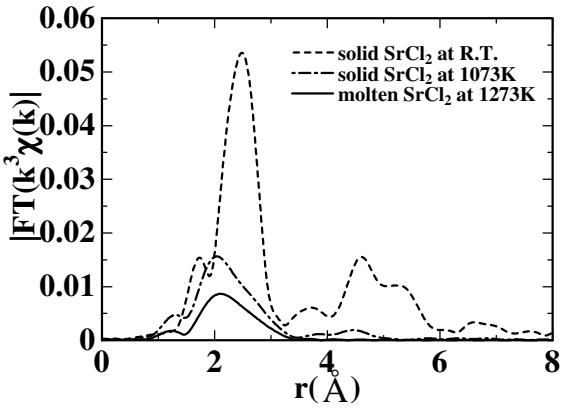

Fig.1 XAFS function $k^3\chi(k)$ and Fourier transform magnitude |FT| of $SrCl_2$

Table 1 Structural parameters (N: coordination number, r: interionic distance, σ^2: Debye-Waller factor, C3,C4: 3rd and 4th cumulants) of the nearest Sr^{2+}-Cl^- correlation in $SrCl_2$

	N	r(Å)	σ^2(Å^2)	C3(Å^3)	C4(Å^4)
R.T.	8.0(fix)	3.00	0.0159	---------	--------
1073K	8.1	3.07	0.0416	8.5×10^{-3}	7.1×10^{-4}
1273K	6.6	2.99	0.0574	6.8×10^{-3}	1.5×10^{-3}

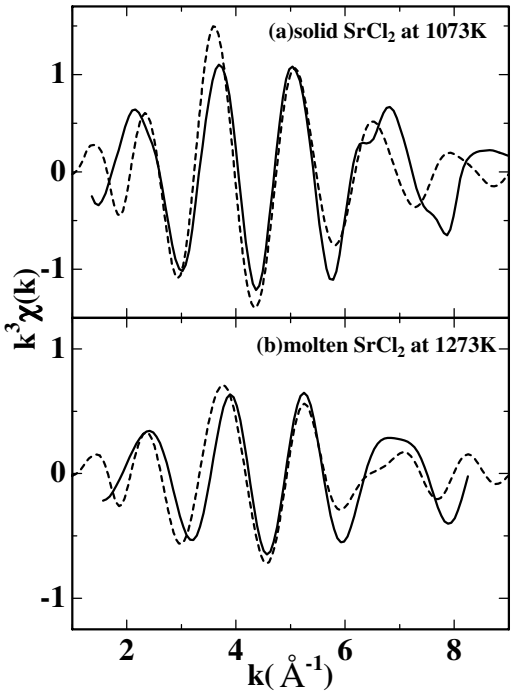

Fig.2 XAFS function $k^3\chi(k)$
solid : experimental, dashed : MD+GNXAS

References

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* okamoto@molten.tokai.jaeri.go.jp