Dynamic and static disorder of alkali halide solid solutions studied by temperature-dependent extended X-ray-absorption fine structure

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Introduction

A solid solution is a material which is composed of a mixture of atoms or molecules over a range of compositions, and still remains in a single phase. Solid solutions have attracted wide attention not only for fundamental science but also for technological applications, because their properties can be controlled by changing the composition. Although the structures of solid solutions have been well studied and understood, the interatomic potential of solid solutions has not been well understood so far. In the present study, we have studied the interatomic potential of alkali halide solid solutions using temperature dependent EXAFS measurements.

Experiment

$KCl_{0.8}Br_{0.2}$ and $KBr_{0.2}I_{0.8}$ were prepared by mixing appropriate amounts of KBr and KCl or KI, followed by repeated treatments of grinding and melting. Br K-edge EXAFS spectra of the solid solutions and KBr were taken by means of the conventional transmission mode at BL-10B in the Photon Factory of the Institute of Materials Structure Science.

Results and discussion

Fig. 1 shows the fourier transform of Br K-edge EXAFS functions of $k^2\chi(k)$ at 32 K, 100 K and 200 K for KBr, $KCl_{0.8}Br_{0.2}$ and $KBr_{0.2}I_{0.8}$. The K-Br bond length and the Einstein temperatures of the K-Br bond for solid solutions were determined by means of the curve-fitting method. The numerical results are shown in Table I. The K-Br bond was contracted by 0.06 Å for $KCl_{0.8}Br_{0.2}$, while it was elongated by 0.09 Å for $KBr_{0.2}I_{0.8}$, as compared to that in KBr. The Einstein temperature decreased with the K-Br bond length, that is, the longer K-Br bond was softer than the shorter K-Br bond. Since the K-Br interatomic potential is anharmonic, the second derivative of the interatomic potential decreases with an increase in the bond length. Therefore, the force constant, that is, Einstein temperature, decreased with the bond length. The static disorder and dynamic disorder could be analysed separately within the Einstein approximation. If the concentration of KBr is low, the static disorder of the K-Br bond in solid solutions was not always larger than that for bulk KBr. The static disorder also increased with the bond length.
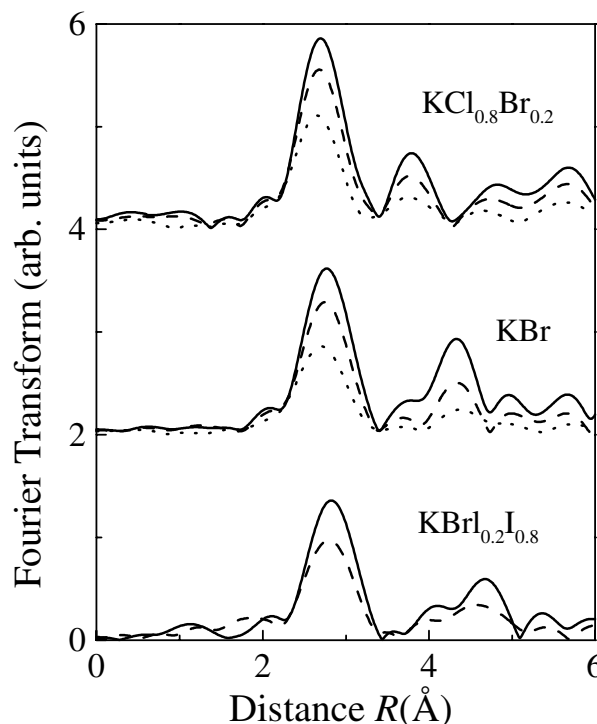

Fig. 1 Fourier transform of Br K-edge EXAFS function of $k^2\chi(k)$ at 32 K (full line), 100 K (dashed line) and 200 K (dot line) for $KCl_{0.8}Br_{0.2}$, KBr and $KBr_{0.2}I_{0.8}$.

Table I: The K-Br bond length and Einstein temperature (ϑ_E) of the K-Br bond for KBr, $KCl_{0.8}Br_{0.2}$ and $KBr_{0.2}I_{0.8}$.

System	R (Å)	ϑ_E (K)
KBr	3.26(2)	155(5)
$KCl_{0.8}Br_{0.2}$	3.20(2)	170(5)
$KBr_{0.2}I_{0.8}$	3.35(2)	130(5)

References

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