Relationship between thermal conductivity and structure for the alkaline earth boroalminate melts

S. Yamada[1], K. Morita[1], A. Nakayama[2] , H. Aoki[3]
1. Department of Materials Engineering, Graduate School of Engineering, The University of Tokyo
2. Nippon steel Corporation
3. JFE Steel Corporation

1 INTRODUCTION

Mold flux regulates the cooling rate of the molten steel's surface to prevent cracking, thus enhancing the quality of steel products. The thermal conductivity of mold flux is crucial. Regarding the modifier effect, the molar volume of the crystal containing CaO and MgO is not independent of the proportion of Ca to the alkaline earth metal. And the effects of composition on the thermal conductivities of fluxes containing $BO_{1.5}$ and $AlO_{1.5}$ were not thoroughly understood due to their complex structures.

Components of mold flux (example)

CaO	SiO_2	$AlO_{1.5}$	$BO_{1.5}$	MgO	Na_2O
Network modifier	Network former	both	Network former	Network modifier	Network modifier

2 METHODS

Thermal conductivity	
Hot wire method	
T(K)	1573-1773
Structure analysis	
Raman spectrometry	
signal(cm^{-1})	400-1600
MAS-NMR	
^{11}B, ^{27}Al , ^{29}Si	

Glass samples used for structure analysis was made with melting at 1773 K and quenched.

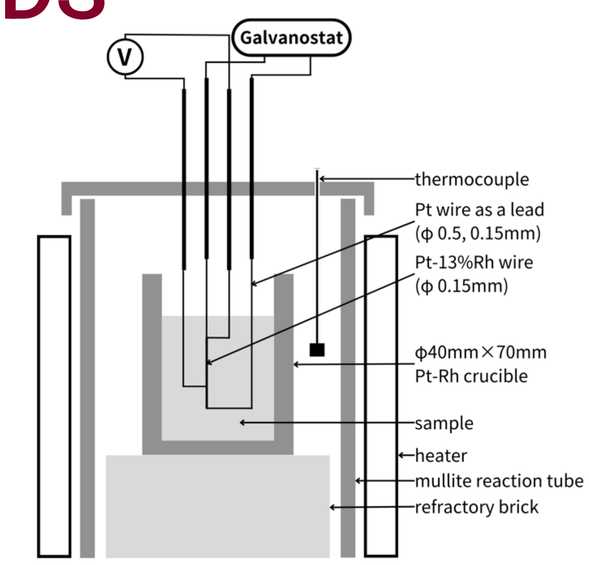

Fig. Experimental setup for thermal conductivity measurement

3 RESULTS & DISSCUSSION

The thermal conductivity and structure of the molten CaO-$AlO_{1.5}$-$BO_{1.5}$ system

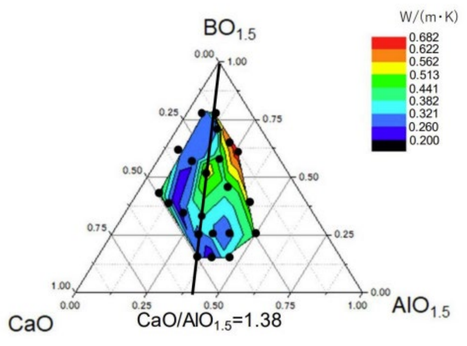

Fig. thermal conductivity of CBA

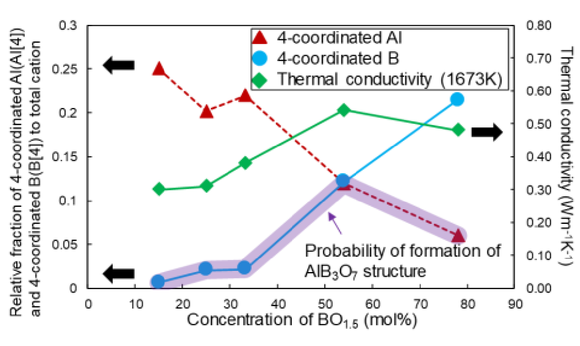

Fig. relative fractions of Al[4] and B[4] for the CBA

low $BO_{1.5}$ range → Al[4] acts as network former.

high $BO_{1.5}$ range → B[4] acts as network former.

▶ AlB_3O_7 structure contributes to heat conduction in the CBA system.

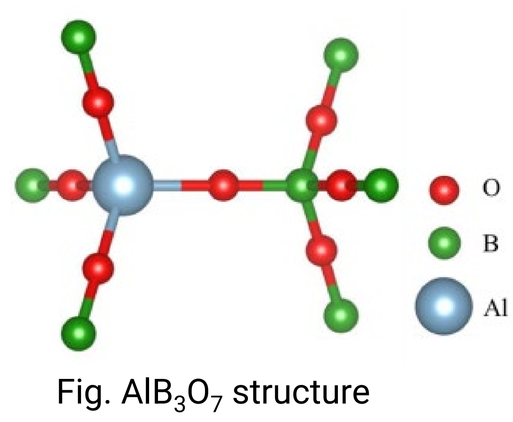

Fig. AlB_3O_7 structure

Amount of AlB_3O_7 structure depend on

when low $BO_{1.5}$ range → Al[4]

when high $BO_{1.5}$ range → B[4]

the large unit of AlB_3O_7 structure makes the conductivity of the heat by the phonon conduction better.

Covalency of the network of molten oxide evaluated using first principle calculations

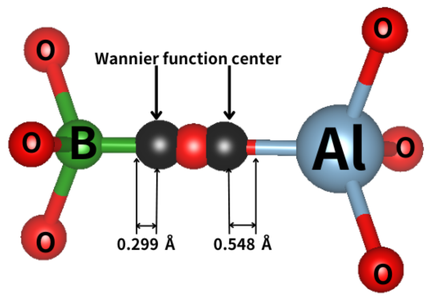

Fig. Wannier function center and D of B[4]-O-Al[4]

$$D_{ave} = \frac{\sum_i X[n]_i n \mathrm{L}(X[n]_i)}{\sum_i X[n]_i n}$$

$$S = \sqrt{\frac{\Sigma_{M[n]}\left(D_{M[n]} - D_{ave}\right)^2 \times n \times X_{M[n]}}{\Sigma_{M[n]}\left(n \times X_{M[n]}\right)}}$$

$$BO\% = \frac{O_{total} - NBO}{O_{total}}$$

Table. D of X-O bond in X-O-Y(Å)

X \ Y	B[4]	Al[4]	Al[6]
B[4]	0.317	0.299	0.417
Al[4]	0.548	0.532	0.705
Al[6]	0.604	0.600	0.571

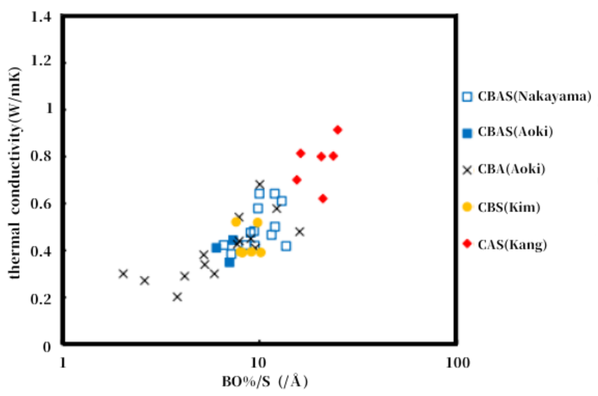

Fig. thermal conductivity & BO%/S

When BO%/S was up, thermal conductivity was also up.

this tendency was able to confirm in many systems.

Mixed modifier effect on thermal conductivity of the molten CaO-MgO-$AlO_{1.5}$-$BO_{1.5}$ system

Thermal conductivity exhibited a local minimum with the increase of MgO.

R=[MgO]/([CaO]+[MgO])

→Mixed modifier effect

Table. fraction of CMBA

CaO+MgO	R	$BO_{1.5}$	$AlO_{1.5}$
27mol%	0, 0.35, 0.51, 0.68, 1	54mol%	19mol%

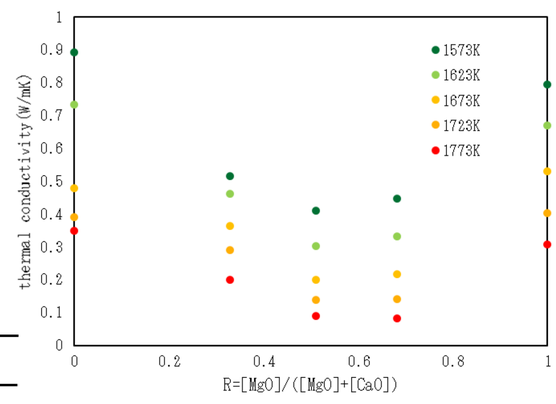

Fig. thermal conductivity & R

4 CONCLUSION

- The AlB_3O_7 structure contributed to an increase in thermal conductivity.
- The relationship between thermal conductivity and structure could be quantitatively evaluated using BO%/S, a combination of the variation in the degree of polymerization BO% and its covalency in the network structure S.
- A mixed modifier effect is observed on the thermal conductivity of molten oxides containing CaO and MgO.