Physical properties and polymorphism of F-containing rare-earth fluorite-like molybdates with structure $Nd_5Mo_3O_{16}$ type doped with sodium

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HE-fuel cells-Poster

INTRODUCTION

The binary Ln_2O_3-MoO_3 systems are of interest because some compounds in such systems have high oxygen or mixed conductivity[1,2]. The $Ln_5Mo_3O_{16}$ (5:6) compounds have cubic fluorite-like structure and mixed oxygen and electronic conductivity[2,3]. Faurie[4] expanded the family of fluorite-like compounds by replacing one rare-earth element with one-valent alkaline element and one oxygen atom with fluorine. This work is devoted to study of physical properties of $NaLn_4Mo_3O_{15}F$ compounds (Ln=La,Pr,Nd).

EXPERIMENTAL/THEORETICAL STUDY

Polycrystalline samples $NaLn_4Mo_3O_{15}F$ (Ln=La,Pr,Nd) were obtained by solid state reaction method in air at 700°C. XRD characterization was performed with DRON-2.0 diffractometer (CuKα-radiation). Differential scanning calorimetry (DSC) has been made using NETZSCH STA 449C. Temperature dependences of conductivity and dielectric permittivity were measured using special impedance spectrometer[5].

RESULTS AND DISCUSSION

$NaLn_4Mo_3O_{15}F$ (Ln=La,Pr,Nd) compounds have cubic fluorite-like structure with Pn-3n space group. DSC reversible peaks were observed near 600 °C under heating and cooling. Such anomalies may indicate the existence of a phase transition. It should be noted there was no information about such transition in $Ln_5Mo_3O_{16}$ fluorite-like compounds. A jump in electrical conductivity and an anomaly of permittivity of the ferroelectric type were observed on the temperature dependences of electrical properties, which confirm the existence of the phase transition. Conductivity temperature dependences for $NaLa_4Mo_3O_{15}F$ are shown in Fig. 1. A small hysteresis of the conductivity is observed during heating and cooling. The maximum conductivity is close to 0.032 S/cm at 700 °C. A rather intensive piezoelectric effect was detected in the $NaLn_4Mo_3O_{15}F$ compounds.

The detected phase transition may indicate that the true symmetry of the oxyfluorides $NaLn_4Mo_3O_{15}F$ at room temperature differs from the cubic one. Replacement of one rare earth element with sodium and one oxygen with fluorine should lead to distortion of crystal lattice and the appearance of oxygen vacancies, which may be associated with an increase in conductivity.

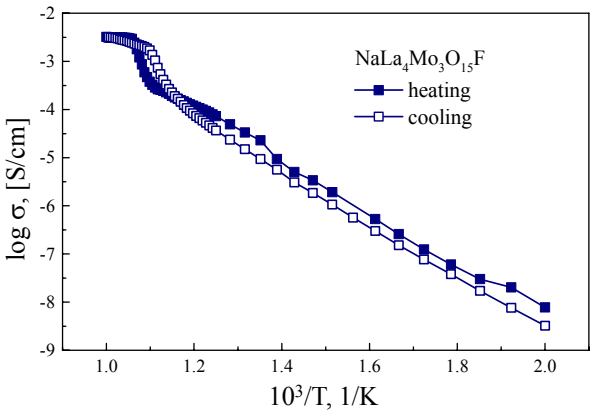

Fig. 1 Conductivity temperature dependence for $NaLa_4Mo_3O_{15}F$ sample

CONCLUSION

Fluorite-like oxyfluorides $NaLn_4Mo_3O_{15}F$ (Ln = La, Pr,Nd) were obtained by solid-phase synthesis in air at 700 °C. Codoping of the $Nd_5Mo_3O_{16}$ family with sodium and fluorine led to the appearance of a piezoelectric effect and a reversible phase transition in oxyfluorides, accompanied by a jump in the conductivity and an anomaly of the permittivity of the ferroelectric type. It is necessary to find out the reason for this phenomenon.

REFERENCES

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