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Investigation on Thermal Expansion of BaY_2F_8 Single Crystal Grown by Temperature Gradient Method

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Abstract

The thermal expansion curve of BaY_2F_8 single crystal was measured in the temperature range from 313 K to 1171 K and the thermal expansion behaviors were also investigated in detail. The thermal expansion is the performance of atomic non-simple harmonic motion. In this paper, the atomic interaction potential is expanded by Taylor's series and the theoretical thermal expansion coefficient was obtained. On a basis of the experimental thermal expansion data, the linear and nonlinear expansion coefficient are obtained through a quadratic curve fitting procedures. Through calculating and analyzing the thermal expansion coefficient, we can better understand the behavior of BaY_2F_8 crystal grown by temperature gradient method.

Keywords: *Thermal expansion coefficient, Taylor' series, Temperature gradient method, BaY_2F_8, Linear fitting curve*

1. Introduction

The thermal expansion coefficient of material is related to the chemical composition, crystalline state, crystal structure and bond strength. Materials with the different structure have different expansion coefficients. Generally, the thermal expansion coefficient of crystal materials is larger than that of amorphous glass and materials with high bond strength usually have low thermal expansion coefficient. The phase transition may occur during crystal growth and the thermal expansion coefficient will also change at the same time [1-3]. The thermal expansion has a great effect on the crystal growth process. Therefore, calculating and analyzing the thermal expansion coefficient are helpful to crystal growth.

Barium yttrium fluoride (BaY_2F_8-BaYF) has important mechanical and thermal features. For example, the very low phonon energy reduces occurrence of non-radiative processes with respect to the radiative ones. In addition, if compared with the refractive index of oxides, the low refractive index of the BaY2F8 single crystal suggests a low thermal lensing effect, which contributes to the luminescence of the activators. In the present work, the thermal expansion curve of BaY_2F_8 single crystal was measured in the temperature range from 313 K to 1171 K and the thermal expansion behaviors were also investigated in detail. The theoretical thermal expansion coefficient was analyzed. On a basis of the experimental thermal expansion data, the linear and nonlinear expansion coefficient are obtained through a quadratic curve fitting procedures.

2. Experimental procedures

The pure BaY_2F_8 single crystal was grown by temperature gradient method [4-5]. High-purity synthesized powders (>99.99%) of commercially available BaF_2 and YF_3 were applied to crystal growth and these raw materials were mixed in stoichiometric amounts according to the following equation:

$$BaF_2 + 2YF_3 \rightarrow BaY_2F_8 \quad (1)$$

The measurement of thermal expansion curve along the [100] direction was carried out with a NETZSCH DIL 402C high-precision dilatometer. The dimensions of the tested sample were 5 mm × 5 mm × 5 mm.

3. Results and discussion

The atom has the lowest energy in the position of equilibrium. When the atom shifts δ to the right from the equilibrium position, the potential energy is $U(r_0+\delta)$. The atomic interaction potential energy can be expanded by the Tayor's series. This formula is as follows:

$$U(r_0+\delta)=U(r_0)+\left(\frac{\partial U}{\partial r}\right)_{r_0}\delta+\frac{1}{2!}\left(\frac{\partial^2 U}{\partial r^2}\right)_{r_0}\delta^2+\frac{1}{3!}\left(\frac{\partial^3 U}{\partial r^3}\right)_{r_0}\delta^3+\frac{1}{4!}\left(\frac{\partial^4 U}{\partial r^4}\right)_{r_0}\delta^4\cdots \quad (2)$$

Where the $U(r_0)$ is atomic lowest potential energy, it can be used as zero potential energy. The second term equals zero in Eq. (2), which means that there is only kinetic energy when the atom is in equilibrium position. The fourth term is the anharmonic term of atoms repelling each other. The fifth term will reflect the relationship between crystal expansion and temperature. Now, we make the third, fourth and fifth terms equal to *f*, *-g* and *h*, respectively. The atomic interaction potential energy can be given by following equation:

$$U(r_0+\delta)= f\delta^2-g\delta^3+h\delta^4 \quad (3)$$

It is noted that the average displacement of atom follows a Boltzmann type population distribution. The average atomic displacement can be expressed as follows:

$$\delta=\frac{\int_{-\infty}^{+\infty}\delta e^{U/K_BT}d\delta}{\int_{-\infty}^{+\infty}e^{U/K_BT}d\delta} \quad (4)$$

As seen from Eqs. (4) and (3), the average atomic displacement is approximate to the following formula:

$$\delta=\frac{3gk_BT}{4f^2-3hk_BT} \quad (5)$$

The coefficient of linear expansion in the single crystal can be defined by following formula:

$$\beta=\frac{1}{r}\frac{d\delta}{dT}=\frac{12f^2gk_B}{r_0\left(4f^2-3hk_BT\right)^2} \quad (6)$$

In this paper, we apply the short-range potential model called Morse potential, which is expressed as follows:

$$U(r)=D\left(1-e^{-\alpha\delta}\right)^2 \quad (7)$$

The atomic interaction potential is expanded by the Taylor's series. These parameters are given by following equations:

$$f=D\alpha^2 \quad , \quad g=D\alpha^3 \quad , \quad h=\frac{7}{12}D\alpha^4 \quad (8)$$

Substituting Eqs. (8) into Eqs. (7), the thermal expansion coefficient in the single crystal can be defined by following formula:

$$\beta = \frac{192Dk_B}{\alpha r_0 (16D - 7k_B T)^2} \quad (9)$$

Where β is thermal expansion coefficient. k_B is the Boltzmann constant, which is equal to 1.38×10^{-23}. r_0 is the equilibrium position of atoms and we choose the distance between two F^- ions (about 2.750 Å). D and α are the parameters of the linear expansion coefficient calculation. Based on the Eq. (9), the value of the thermal expansion coefficient β is about 3.7261×10^{-5} K^{-1}, which is much larger than the standard value (~ 1.8×10^{-5} K^{-1}). BaY_2F_8 single crystals belong to the monoclinic crystallographic system, which means that the symmetry of BaY_2F_8 crystal is very low and the whole calculation process must be corrected. The Eq. (9) is only an approximate calculation process [6-8].

In order to obtain an accurate thermal expansion coefficient, the thermal expansion curve along the [100] direction was measured in the temperature range from 313 K to 1191 K, as shown in Fig. 1. These data were analyzed by linear regression and quadratic regression, respectively. The purpose of quadratic regression analysis is to evaluate the matching degree of thermal expansion curve. The linear regression and quadratic regression function can be given as follows:

$$\frac{\Delta L}{L} = C + \beta T \quad (10)$$

$$\frac{\Delta L}{L} = C + \beta_1 T + \beta_2 T^2 \quad (11)$$

Where C is the fitting constant, β is the linear thermal expansion coefficient and β_1 and β_2 are first-order fitting coefficient and second-order fitting coefficient, respectively. The first-order coefficient (β_1) represents the steepness of the curve and second-order coefficient (β_2) represents the bending depth of the curve. The theoretical and experimental fitting parameters are listed in Table 1. Compared with theoretical calculation and quadratic regression, the linear regression is more consistent with the experimental thermal expansion curve.

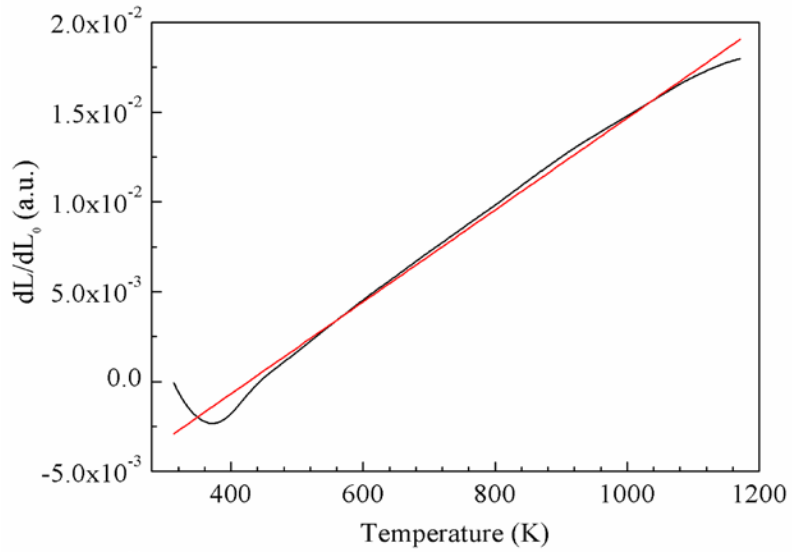

Fig. 1. Thermal expansion curve along the [100] direction

Table 1. Values of theoretical and experimental fitting parameters

Theoretical calculation	Linear regression		Quadratic regression		
β ($\times 10^{-5}$)	C	β ($\times 10^{-5}$)	C	β_1 ($\times 10^{-5}$)	β_2 ($\times 10^{-5}$)
3.7261	0.01049	2.1333	-0.0238	5.7387	-1.9098

As can be seen from Fig. 1, the red line is a linear fitting curve, which is not in good agreement with the experimental expansion curve in the temperature range from 1100 K to 1170 K. This phenomenon suggests that a large relative deformation exist in the BaY2F8 crystal. According to the phase diagram of the BaF_2-YF_3 systems (as shown in Fig. 2) [9], the $\alpha \rightarrow \beta$ phase transition occurs in the same temperature range below the melting temperature. In order to make the crystal undergo the relative deformation and $\alpha \rightarrow \beta$ phase transition stage, the final cooling rate must be reduced in the crystal growth process.

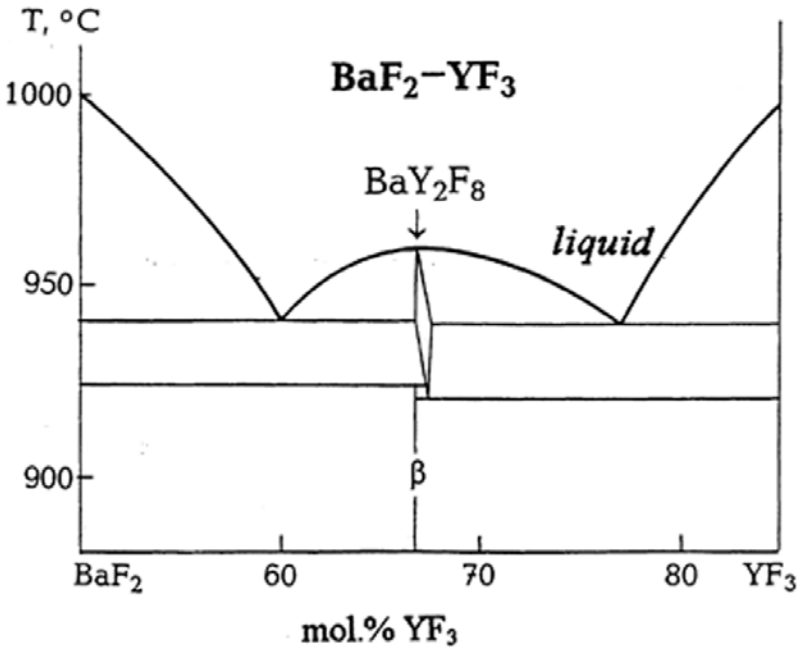

Fig. 2. Phase diagram of BaF_2-YF_3 system

4. Conclusions

In summary, the thermal expansion curve of BaY_2F_8 single crystal was measured in the temperature range from 313 K to 1171 K and the thermal expansion behaviors were also investigated in detail. Theoretical thermal expansion coefficient was obtained. On a basis of the experimental thermal expansion data, the linear and nonlinear expansion coefficient are obtained through a quadratic curve fitting procedures. Through calculating and analyzing the thermal expansion coefficient, we can better understand the behavior of BaY_2F_8 crystal grown by temperature gradient method.

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