Data Article

Dataset for correlation in $\gamma$-RbAg$_4$I$_5$ between ionic conductivity relaxation and specific heat

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**ABSTRACT**

Using the ac-calorimetry technique and the electric modulus formalism for analysis of ionic conductivity relaxation in crystalline $\gamma$-RbAg$_4$I$_5$, close to the $\gamma$ to $\beta$ phase transition at 120 K, the temperature derivative of microscopic interaction energy for a single-mobile ion is proportional to the specific heat. The two different experimental techniques show that cooperative behavior drives the phase transition at 120 K (obey the same mechanism).

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1. Data

Fig. 1 shows a discontinuous change of the dc-conductivity with an associated peak in the excess specific heat of RbAg$_4$I$_5$ where the first-order phase transition occurs at 120 K or phase boundary is between the $\gamma$- RbAg4I5 and $\beta$- RbAg4I5 $[1–3]$. The value of enthalpy corresponding to the phase transition is provided by the migration energy, which allows us to correlated both thermodynamics and transport concepts.

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2. Experimental design, materials and methods

Using the solution technique with high purity reagents [4], the RbAg₄I₅ crystals at 318 K and dried at 390 K for about 6 hours were grown. For the crystallographic analysis, the crystal samples are a representative specimen.

Using the ac-calorimetry technique [5,6], the specific heat data of RbAg₄I₅ single crystals were continuously obtained. Using dry abrasives crystal slices were thinned to 0.1 mm. By light chopped at 1.5 Hz, the sample was heated. Using a 25 \( \mu \)m type-K thermocouple, the temperature oscillations induced in the sample, inversely proportional to the specific heat, were monitored. The sample was

![Fig. 1. The specific heat at a constant pressure of RbAg₄I₅ as a function of temperature. At 120 K, the first-order phase transition occurred.](image)
swept slowly through the region of the phase transitions to obtain the specific heat at constant pressure $c_p(T)$ as a function of the temperature $T$.

Using the two-electrode configuration Ag|RbAg$_4$I$_5$|Ag with silver paste as electrodes, an electrical measurement was made. By admittance spectroscopy in 20 Hz to 3 MHz frequency range, using a precision LCR meter HP 4284A and at different fixed temperatures between 105 K and 121 K, under a dry nitrogen atmosphere, the electrical characterization was done. The amplitude of the applied ac signal was 10 mV.

In the crossover region, the dependence of the real part of the ac conductivity $\sigma'(T, \omega)$, is described for ionic conducting materials by a power law [7]:

$$\sigma'(T, \omega) = \sigma_0(T) \left[ 1 + \left( \frac{\omega}{\omega_p(T)} \right)^n \right]$$

(1)
where $\omega_p$ is a characteristic relaxation, $\sigma_0$ is the dc conductivity, and $n$ is the power-law exponent related to the degree of correlation among moving ions [8]. The frequency dependence of the real part of the ac conductivity for isotherms in the 116 k to 124 K temperature range is shown in Fig. 2.

The parameters $\omega_p(T)$ and $\sigma_0(T)$ were obtained by fitting the $\sigma(\omega)$ data at various isotherms according to

$$M^*(\omega) = \frac{1}{\varepsilon^*(\omega)} = \frac{i\varepsilon_0}{\sigma^*(\omega)}$$

(2)

and the Arrhenius plot [log($\sigma_0$) as a function of 1000/$T$] is shown in Fig. 3.

Activation energy, $E_{act} = \partial\ln(\sigma_0)/\partial(1/T)$, is non-Arrhenius in the 118.4 k to 119.8 K temperature range for dc-conductivity data.

Frequency dependence of the imaginary part of the dielectric modulus is shown in Fig. 4 at several temperatures range (117.5 K and 119.8 K):

Fig. 4. Dependence of frequency of the real part of the electrical modulus for 117.5 and 119.8 K temperature range.

Fig. 5. $\beta$-correlation function, the activation, microscopic and migration energies as a function of temperature.
The $\beta$-correlation function, the activation, microscopic and migration energies as a function of temperature is shown in Fig. 5 for 117.5 K and 119.8 K temperature range. Results of $d(\beta E_{\text{act}})/dT$ and $D_{cp}$ is shown in Fig. 6 where these quantities exhibit similar behavior with temperature.

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Conflict of Interest

The authors declare that we have no known competing financial interests or personal relationships that could have appeared to influence the work reported in our paper.

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