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Behaviour of Nano-crystalline Scandium Oxide under the Extreme Condition

Neha Bura (1,2), Jasveer Singh (2) ,Deepa Yadav (1,2), Ankit (1,2) and Nita Dilawar Sharma (1)
(1) Academy of Scientific and Innovative Research, Ghaziabad-201002, India.
(2) CSIR-National Physical Laboratory, Dr. K.S. Krishan Marg, New Delhi-110012, India.

Abstract

We present the temperature dependent variation of phonon modes in nano-crystalline Scandium Oxide (Sc_2O_3) for the temperature range of 80K-440K. The structural stability of the nano-sized oxide with the temperature is studied and the phonon modes were observed to shift to lower wavenumbers with increase in temperature. The anharmonic constants were determined along with phonon lifetimes. The DSC measurements were also done to investigate the phase transition temperature.

Introduction

The study of the materials under the extreme conditions have become an important area of study to explore the variations in the structure and property related to the applied temperature and pressure, which directly impact the applications of these materials and hence their performance. The Rare Earth Sesquioxides are studied due to their applications in Nuclear Reactor, Nuclear waste host materials and many more. In this paper we have studied the Sc_2O_3 under the extremes of the temperature i.e. from 80K to 440K using the Raman Measurements.

1. Experimental Method

The sample with the 99.9% of purity was used as the starting material. For the low temperature measurement a pellet of diameter 3mm was made. The sample was loaded in the sample chamber of the continuous flow cryostat and laser was focused on the sample with the 20X objective. A Jobin Yvon made triple Raman Spectrometer with the excitation wavelength of 514.5nm was used for the Raman Measurements.

1.1 Preliminary Studies on Material

The XRD, SEM and EDS Measurements were done on the sample. The Results from the XRD analysis show that sample is in cubic phase with the crystallite size of the 34 nm. Surface morphology of the sample was found out using the SEM measurements. The purity of the sample was confirmed by the EDS measurements.

2. Figures

The Figure 1 shows the Raman Spectra of Scandium Oxide with the varying temperature. The variation in the width of the peaks and the shift in the peak position is clearly visible in the graph.

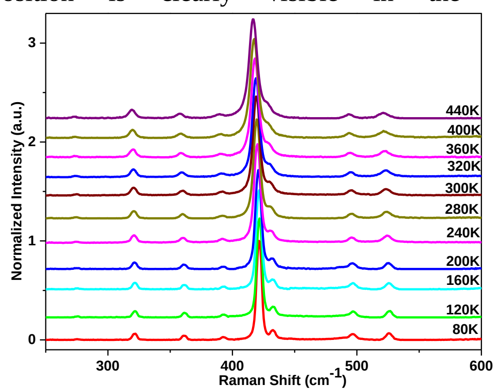

Figure 1: Raman Spectra for increasing Temperature.

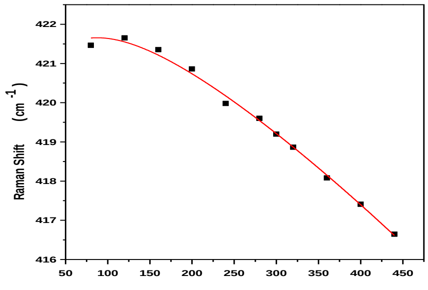

Figure 2: Variation of Frequency with the temperature.

Figure 2 shows the variation in the frequency of the Peak for the peak observed at 419.3 cm^{-1} with the temperature. The graph is fitted with the equation 1 and values of anharmonic constants, A and B comes out to be -4.04 cm^{-1} and -0.09cm^{-1} respectively. The negative values of anharmonic constants indicate the phonon softening with the temperature. Higher value of A indicates predominance of three phonon process

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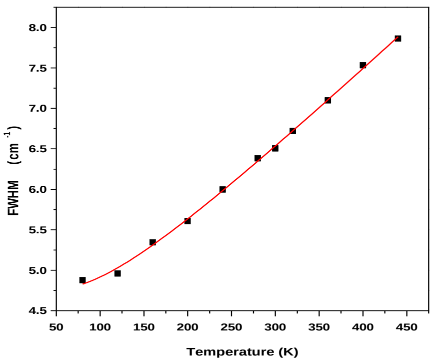

Figure 3: Variation of FWHM with the varying Temperature

The graph full width of half maxima v/s temperature for the peak observed at 419.3 cm^{-1} is fitted with the equation 2 and value of anharmonic constants i.e. C and D is found to be 1.49 cm^{-1} and 0.02 cm^{-1}. The positive values of anharmonic constant implies the broadening of the peaks with the temperature.

3. Tables

Raman Modes (cm^{-1})	**Assignment**
221.6	**A_g**
359.7	**$E_g + F_g$**
393.0	**$A_g + F_g$**
419.2	**F_g**
495.8	**$A_g + F_g$**
523.8	**F_g**

The Table shows the Identification of Various Raman modes.

4. Equations

The equations used to fit the data of Raman Shift v/s Temperature and Full width of half maxima v/s Temperature are given below.

The Frequency at any temperature is the sum of harmonic frequency and frequency shift due to the anharmonicity as well as thermal effects.

$$\omega(T) = \omega + (\Delta\omega)_{latt} + (\Delta\omega)_{anh} \quad \ldots\ldots\ldots\ldots\ldots (1)$$

The $(\Delta\omega)_{latt}$ represents the contribution in frequency due to the thermal expansion.

$$(\Delta\omega)_{latt} = \omega_0\{\exp[-\gamma_i \int_0^T 3\alpha(T)dT] - 1\}$$

α represent the thermal expansion coefficient and γ represent the mode Grüneisen parameter.

The $(\Delta\omega)_{anh}$ arises from the pure temperature contribution and is given by

$$(\Delta\omega)_{anh} = A[1 + \frac{2}{\exp(\hbar\omega_0/2kT) - 1}] + B[1 + \frac{3}{\exp(\hbar\omega_0/3kT) - 1} + \frac{3}{(\exp(\hbar\omega_0/3kT) - 1)^2}]$$

The 1st term of the equation comes from the three phonon process and 2nd term comes from the four phonon process.

The variation of FWHM with the temperature is given by the equation

$$\Gamma = \Gamma_0 + C[1 + \frac{2}{\exp(\hbar\omega_0/2kT) - 1}] + D[1 + \frac{3}{\exp(\hbar\omega_0/3kT) - 1} + \frac{3}{(\exp(\hbar\omega_0/3kT) - 1)^2}] \quad \ldots\ldots\ldots\ldots\ldots (2)$$

The 2ND and 3rd term represent the contribution from the three phonon process and four phonon process respectively.

A, B, C and D are anharmonic constants.

5. Summary and Conclusions

The Sc_2O_3 shows phonon softening with increase in temperature with a total shift of ~6cm^{-1} over the temperature range studied. The anharmonicity analysis shows that this can be attributed to dominance of three phonon interaction. With the increase in temperature the FWHM increases or the phonon life time decreases as the latter is inversely proportional to the former.

Acknowledgements

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