# Effect of Annealing on Phase Transition and Its Impact on Second Harmonic Generation in Barium Titanate Nanopowder for DSSC Solar Cell Applications

S. Mahalakshmi [1, 2], V. Ragavendran [2], V. Vishnukanthan [3, 4], J. Mayandi [2]

[1]*Department of Physics, R.D. Govt. Arts College, Tamilnadu, Sivaganga, India*
[2]*Department of Material Science, School of Chemistry, Madurai Kamaraj University, Tamilnadu, India.*
[3]*Department of Physics/Centre for Materials Science and Nanotechnology, University of Oslo, Oslo, Norway*
[4]*Department of Materials Science, National Research Nuclear University "MEPhI", Moscow, Russian Federation*
*Email: mahaphysics05@gmail.com*

## Abstract

Barium titanate ($BaTiO_3$) nanoparticles synthesized at 200 °C by sol- hydrothermal process demonstrated stabilization of orthorhombic and tetragonal phases. The influence of annealing at different temperatures (100, 200, 300, 400, 500 & 800 °C) on the phase separation/transition is investigated in this study. The annealing process had substantial impact on the structural and phase variation in $BaTiO_3$ nanopowder as observed from XRD analysis. An evident phase transition from the orthorhombic to the tetragonal phase is observed when the $BaTiO_3$ nanoparticles are annealed at 100°C and tetragonal phase along with orthorhombic phase is observed for all other annealed samples. Annealing at 800 °C resulted in stabilization of pure rhombohedral phase. Surprisingly, dominating XRD peaks (NP) were observed in annealed samples at 100 – 400 °C, often related to $BaCO_3$ in literature, even though barium (II) chloride, titanium (IV) chloride and NaOH were used as the precursors. The nanoparticles were further characterized by SEM and TEM, which showed uniform spherical shaped nanoparticles transformed to rod morphology with increase in agglomeration of particles. Raman Spectroscopy analysis showed the presence of characteristic tetragonal and orthorhombic Raman bands and the annealed materials exhibited similar characteristics as that of as-synthesized material, in addition, it shows an additional sharp peak around 690 $cm^{-1}$, identified as corresponding to hexagonal phase in literature, suggests new phase transition or phase separation in $BaTiO_3$. These results coincide well with UV and PL spectrum analysis. All the samples demonstrate non-linear optical properties demonstrating second harmonic generation. Identification of the NP-XRD peaks and influence of annealing on the second harmonic generation are presented in detail. Finally, Dye-sensitized solar cell with $BaTiO_3$ as photo anode will be fabricated and its IV characteristics will be studied.