The Effect of Transition Metal Dopants on the Physical Properties of Perovskites Studied by XRD Analysis

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Abstract. The minerals, commonly called Perovskites, were discovered in the Ural Mountains in 1839. These new compounds have a chemical formula derived from or very similar to the original formula, ABX3. Perovskite compounds are ionic in nature.The importance of Perovskites increased significantly after the discovery of the dielectric and ferroelectric properties of barium titanate, BaTiO3, in the 1940s. As a result, the material quickly found applications in electronics in the form of capacitors, sensors and transducers. Extensive research on these materials includes extensions to phases having nitride or oxonitride ions. These materials are becoming of considerable importance in the fields of electrical ceramics, refractories, geophysics, materials science, astrophysics, particle accelerators, heterogeneous catalysis and the environment. Therefore, Perovskites have become one of the worldwide studied materials due to their special properties such as ferroelectric, thermoelectric, pyroelectric, dielectric and optical properties. Most natural photoelectric materials have limitations for use in photovoltaic applications. This is their band structure with a gap size in the valence band. To shift the range of usable radiation, these materials need to be doped. The doping of transition metals such as Ni, Fe and Cr can be advantageously used, which have been found to have a significant effect on improving the physical properties of these materials.

The aim of this work is the use of transition metal doped STO in photovoltaic applications. The essence of the present work is to assess the effect of dopants on the structural and electronic properties of the well-known STO perovskite. The use of dopants, preferably transition metals, affects the physical properties in the sense of exploiting favorable pristine properties that are limited by too large a gap in the valence band. Thus, it is a question of assessing the effect of these transition metals on crystallinity, the magnitude of the vitric stress, the distribution of the electron-hole pair in the valence band and the shift of the usability of the electromagnetic spectrum into the visible region. The effect of transition metals on the structural and electronic properties of STO will be assessed, with nickel (Ni) taking a priority place in the impact assessment. Another element for which the effect on the above properties will be investigated will be yttrium (Y).