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Structural and electrical properties of Li-doped TiO_2 rutile ceramics

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Abstract - Ceramics of Li doped TiO_2 rutile with concentration between 0 x 0.02 has been synthesized by a solid state reaction method. The structural was studied using x-ray technique. The dc conductivity ($ó_{dc}$), obtained by impedance spectroscopy, has been studied over the temperature range between 400 to 650 ^oC. The lattice parameters, $ó_{dc}$ and E_a dependence with Li doping show a change in its behavior with the dopant level increase. This effect of Li incorporation is interpreted in terms of two different defects reaction mechanisms. For 0 x 0.01 Li incorporate into interstitial site, while for higher concentrations (up to x 0.02) Li substitutes for Ti in the tetragonal structure, favouring the formation of complex defects.

TiO_2 ceramics have been widely investigated owing to their broad range of applications in different fields [1,2]. In the present work, the structural and electrical properties of the ceramic system TiO_2 + x Li, where 0 x 0.02 is the mole fraction, are showed. The X-ray diffraction analysis shows experimentally that: *i*) the TiO_2 rutile-type structure can incorporate lithium ions up to x=0.02 and *ii*) some results in disagreement with previous simulations reports [3] are found. Moreover, the X-ray diffraction and the electrical behavior have shown that two different defects reaction mechanism for Li ions incorporation in the structure may be happening. The first mechanism, for the low dopant range, is associated with the interstitial Li incorporation. Consequently, a lattice expansion is registered and the ó increasing and the E_a decreasing when the Li concentration is increased. For higher dopant levels, Li substitutional incorporation in Ti-site occurs and mechanism of complex defects formation are suggested. In this dopant range both electrical parameters remain almost constant. The limit for the interstitial to substitutional incorporation is proposed to be x = 0.01.

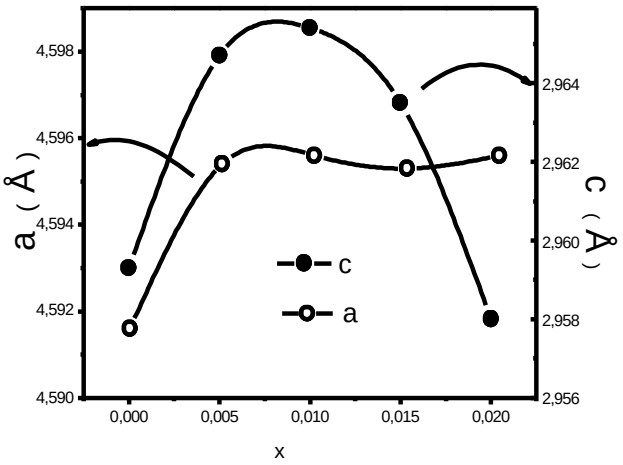

Fig. 1 Li fraction dependence of the *a* and *c* lattice parameters for the tetragonal symmetry of Li doped TiO_2.

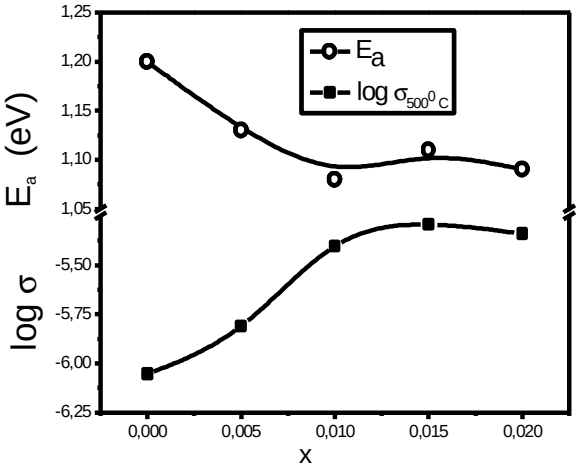

Fig. 2 Effect of the Li doping level on the ionic conductivity $ó_{500}$ (squares) and activation energy, E_a, (circles) of the TiO_2 at 500 ^oC.

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