Research Article

Preludes to the Lattice Compatibility Theory LCT:
Urbach Tailing Controversial Behavior in Some Nanocompounds

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We try to give an explanation to the unexpected Urbach tailing associated to some phenomena which occur in some nano-compounds lattices. The provided discussion and notes are detailed here as a prelude to the lattice compatibility theory (LCT), a guide to a plausible understanding of this unsolved intrigue.

1. Introduction

Urbach tailing alterations inside nanostructured lattices (Figure 1) have been always attributed to atomic-scale topological disorder, unexpected hybrid excitonic transitions, or topological filament occurrence [1–4]. In the beginning of the last decade, Urbach tailing has been attributed to the hydrogen content, and precisely the different E_{04} and sp^2 contents inside nanofilms [5]. Another more realistic explanation has been provided earlier by Dow and Redfield [6]. This explanation claims that Urbach tailing is due to the broadening of the exciton absorption band which occurs when charged impurities in the lattice induce phonon-induced microelectric fields. This phenomenon has been also described, in II–VI compound semiconductors, as a reduction of holes-electrons Coulombic interactions which results in more free excitons, as long as exciton radii are larger than those of alkali halides. Many other causes have been proposed in the relevant literature [7–10].

In this paper, a prelude to the micro-chemistry-related Lattice Compatibility Theory (LCT) is provided as an attempt to explain Urbach tailing alterations in nano-structured lattices. The study is organized as follows. In Section 2, the experimental details and motivations are presented along with the studied nanomaterials patterns. In Section 3, the fundamentals of the proposed Lattice Compatibility Theory LCT are discussed. Last section is a conclusion which summarizes the aim methods and perspectives of the work.

2. Experimental Details and Motivations

In this study, targeted nano-materials are some bismuth oxides BSO, BGO, and BTO. These nano-materials are technologically interesting material, because they can function as a Pockels readout optical modulation (PROM) device and photorefractive sensors [11–18]. Crystals of these oxides were grown from highly purified Bi_2O_3, SiO_2 and presintered BGO, and BTO powders using the Czochralski technique [19]. Elaboration was carried out in room atmosphere and the growing temperature was about 1110°C. Doped nanocrystals were prepared with doping content of 0.02 mol.% in the starting melt and the samples were reexcited each optically by UV radiations for photochromatic effect studies.

In order to understand Urbach tailing alteration following doping agent insertion in host structures, Urbach energy \( E_u \) has been determined, for doped and undoped samples through the equations:

\[
\ln(\alpha(h\nu)) = \ln(\alpha_0) + \frac{h\nu}{E_u},
\]

\[
E_u = \alpha(h\nu) \left( \frac{d[\alpha(h\nu)]}{d[h\nu]} \right)^{-1} = h \left[ \frac{d}{d\nu}(\ln(\nu)) \right]^{-1},
\]

where \( \alpha(h\nu) \) represents, for each sample, the experimentally deduced optical absorption profile.
The width of the localized states (band tail energy or Urbach energy \( E_u \)) has been estimated (Table 1) from the slopes of the plots of \((\ln \alpha (\nu))\) versus energy \( \hbar \nu \).

### Table 1: Values of Urbach energy for doped and undoped nanofilms.

<table>
<thead>
<tr>
<th>Nanofilm</th>
<th>( E_u ) (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BSO</td>
<td></td>
</tr>
<tr>
<td>Un-doped</td>
<td>842.4</td>
</tr>
<tr>
<td>Doped</td>
<td>304.5</td>
</tr>
<tr>
<td>BTO</td>
<td></td>
</tr>
<tr>
<td>Un-doped</td>
<td>564.6</td>
</tr>
<tr>
<td>Doped</td>
<td>559.2</td>
</tr>
<tr>
<td>BGO</td>
<td></td>
</tr>
<tr>
<td>Un-doped</td>
<td>448.7</td>
</tr>
<tr>
<td>Doped</td>
<td>430.5</td>
</tr>
</tbody>
</table>

The second is that despite having the same structures as BSO, nano-structured BGO and BTO react differently under doping. In fact, according to the results recorded in Table 1, the important decrease of Urbach energy with doping (\( \approx 60\% \)) reveals an increasing order that occurs in well-crystallized doped bismuth sillenite BSO contrasts unexpectedly the un-doped ones. This change is absent in the case of doped BTO and BGO. As it was postulated that Urbach energy is a material parameter which indicates the shape of transition from the band tail to the mid gap states (Figure 1), a possible cause to this difference can be attributed to the disposition of the doping agent inside the host matrices (Figure 2(a)). In a first possible scheme, \( \text{CuO}_2 \) copper metallic original fcc lattice is incorporated as such inside BSO host matrix (Figure 2(b)). The second scheme is based on the particularities of \( \text{CuO}_2 \) bonding direction \((\pi,0)/(0,\pi)\). It is known \( \text{CuO}_2 \) layers are simply stacked in fourfold symmetry, without other atoms in the crystal. Bond lengths comparison has been favorable to possible adoption to two adjacent O atoms from tetragonal bismuth as edges of \( \text{CuO}_2 \) lattices (Figure 2(c)). Finally, a possible scheme is based on the magnetic properties of the \( \text{Cu}_2\text{O}_3 \) spin lattices (Figure 2(d)). In this case, a consolidated stabilization inside the host structure is implemented by symmetrically sharing B–O bands hexagonal bonds. This stability has been recorded by Troth and Dainty [20]. These searchers confirmed in their studies on holographic interferometry and anisotropic self-diffraction in sillenite nano-materials that Cu–O bounds in \( \text{Cu}_2\text{O}_3 \) edifices are mainly caused by \( 3d^9 \) configuration of the doping agent ion in a tetrahedral field [20]. On the other hand, it has been confirmed [21–25] that BGO and BTO present distorted octahedral the bismuth-oxygen coordination made

![Figure 1: Urbach tails occurrence scheme.](image-url)
up by five oxygen atom and a lone-pair playing the role of the sixth anion. The actually presented Lattice Compatibility Theory (LCT) features are in good agreement with the precedent analyses as well as the notions of lone-pair orbitals, misfit dislocation, and critical layer thickness [26–30]. The disparity and the introduced uncertainty are recorded for BSO, BTO, and BGO nano-materials plea in favor of this theory as long as it explains the lattice compatibility, the interfacial potential energy, and the strain-associated structural accommodation which were monitored exclusively in the case of BSO.

4. Conclusion

In this work we have tried to give a prelude to the Lattice Compatibility Theory (LCT) as an explanatory guide for understanding Urbach tailing features inside some nano-materials. The stability of doping agents in host matrices has been the main fundament to this theory, as it was recorded exclusively in some particular lattices. In order to implement thoroughbred fundamentals to this theory, it is necessary to investigate the growth kinetics of differently doped oxides in terms of interaction between host matrix and doping agents’ intrinsic structures.

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References


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