SIMULATION BY MOLECULAR DYNAMICS OF THE TRAPPING OF CHARGE IN NON CONDUCTIVE MATERIALS

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Abstract

Charge trapping/detrapping phenomena in solid insulators (Magnesium oxide and sapphire) had been studied by the Dynamic molecular method. Simulations were performed to study punctual defects and trapping phenomena at the molecular scale.

According to our model the first steps gave us some satisfied results about punctual defects and the model of simulating trapping seems to be encouraging.

Keywords : Simulation; Dynamic molecular; Non conductive materials; Trapping charge.

1. Introduction

We are interested in solid insulators because of their electrical properties. Our attention is pointed to the dielectric properties, and we are modelling the mechanisms of trapping charges through a numerical model.

Recently many teams try to understand the response of insulators under several conditions of use. They have shown that: in general, electric properties of insulators were linked to the capacity of trapping charges [1]. The space charge theory in physic, joint to the concept of polaron [2] was built to explain the trapping mechanisms in insulators. Since 1990 Blaise [3] had shown that traps are due to the local variation of the susceptibility of the dielectric; called "defect of polarizability". The trapping phenomena produces a deformation of the lattice around the charge. The material is then able to store a huge quantity of energy brought by an external stress.

The purpose of this work is to show how simulation, using the concept of Dynamic Molecular, could help us to characterize defects by determining the energy of their formation, and simulating the way that dielectrics could trap charges.

2. Analytical method

Our goal using the Dynamic Molecular (DM) is to study the evolution of the behaviour of the lattice and its temperature and time dependencies. The main idea of DM is that lattice is built by ions interacting each other through a potential. So we have to follow the trajectories of particles. The interactive potential we have used is the Buckingham-Van der Walls's which expression is:

\[ V_{ij}(r) = \frac{1}{4\pi\varepsilon_0} \frac{q_i q_j}{r_{ij}} + A_{ij} \exp\left( \frac{-r_{ij}}{\rho} \right) - \frac{C_{ij}}{r_{ij}^6}. \] (1)

The Verlet’s algorithm [4] is chosen to carry out the solution of the equations of movement. The system is analyzed through his Hamiltonian:

\[ H(\dot{\vec{p}}, \vec{q}) = K(\vec{p}) + V(\vec{q}), \] (2)

and using Cartesian system, equations of movement are defined by:

\[ \ddot{\vec{r}}_i = \frac{\vec{p}_i}{M_i}, \] (3a)

and

\[ \dot{\vec{p}}_i = -\frac{\partial V(\vec{r}_1, \vec{r}_2, \vec{r}_3, ..., \vec{r}_N)}{\partial \vec{r}_i}. \] (3b)

Since we are interested in studying the lattice with defects and particularly the deformation and polarisation due to the presence of input charges (trapped charges) it is important to understand the dielectric properties of the material.

In fact, it is well known that at low frequencies, the displacement of ions in the electric field is linked to the dielectrics properties, but at high frequencies the motion of ions is too slow and only the rapid displacements of electrons contribute to the polarization [3]. The model of Shell is chosen, in which each ion is represented by a core and a shell. The two entities are linked by a harmonic spring having a fitting parameter \( k \) (constant of the spring) and the polarizability is then defined by:

\[ \alpha = (Ye)^2 / ke_0, \] (4)

where \( e_0 \) is the permitivity of the vacuum and \( (Ye) \) the charge of the shell.
3. Results and interpretations

For our numerical model, first we have validated the choice of the potential of the crystal by determining the energy of cohesion of the lattice. The lattice must be equilibrated. This goal have been achieved in the canonical form. Particle moves in a field of forces and we are following a particle its involving through the lattice. Punctual defects were characterized by determining their energy of formation. Results are listed in the Tables 1 and 2.

<table>
<thead>
<tr>
<th>Defect</th>
<th>Energy of formation(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(V''_{Mg})</td>
<td>36.68</td>
</tr>
</tbody>
</table>

**Table 1**: Energy of the formation of the defects in MgO.

<table>
<thead>
<tr>
<th>Defect</th>
<th>Energy of formation (eV)</th>
<th>Bibliography</th>
</tr>
</thead>
<tbody>
<tr>
<td>(V''_{Al})</td>
<td>54.80</td>
<td>55.1</td>
</tr>
<tr>
<td>(AL'_{i})</td>
<td>-43.64</td>
<td>-39.3</td>
</tr>
<tr>
<td>(V''_{O})</td>
<td>23.42</td>
<td>23.7</td>
</tr>
<tr>
<td>(O'_{i})</td>
<td>-14.28</td>
<td>-13.5</td>
</tr>
<tr>
<td>Frenkel (anion)</td>
<td>4.57</td>
<td>5.1</td>
</tr>
<tr>
<td>Frenkel (cation)</td>
<td>7.66</td>
<td>7.9</td>
</tr>
</tbody>
</table>

**Table 2**: Energy of formation of the defects in Al\(_2\)O\(_3\).

It is known that to create an oxygen vacancy, we need less energy than to create that of aluminium. The energy of formation of an interstitial is less than the vacancy one for any element. We are interested to characterize punctual defects because their presence has to perturbate the lattice. Punctual defects could be an origin of defect of polarizability and locally changes the dielectric constant. The energy of the formation of the polaron is also determined through the method used by L.Shluger and co-workers [5]. Our results are those in Table 3.

<table>
<thead>
<tr>
<th>(Al_2O_3(1))</th>
<th>(MgO(2))</th>
<th>Variation of the energy of the lattice(eV)</th>
<th>Energy of the formation of the polaron(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Small polaron (1)</td>
<td>(2)</td>
<td>19.64</td>
<td>17.25</td>
</tr>
</tbody>
</table>

**Table 3**: Energy of formation of the small polaron in \(Al_2O_3 (1)\) and MgO (2).

For the trapping phenomena we have introduced in the lattice a particle of charge \(-e\), with a mass equal to the mass of the proton and it is supposed as a particle test. This particle attracts cations and it repulses anions. The interactions are modelled by the potential given as follow [6]:

\[
V_{e^-O^+} (r) = Z_i e^2 / r ,
\]

\[
V_{e^-Q^-} (r) = -Z_i e^2 \frac{\text{erf} \left( \frac{r}{R_0} \right)}{r} .
\]

(5)

with \(R_0\) is the atomic radius of cations.

According to our model, the input particle moves more rapidly in MgO than in the sapphire. In other way, deformation is more important in
MgO than in Al₂O₃ lattice. As the particle is moving rapidly, its localization becomes bad. This agrees with experiments shown by N. DAMMAK [7]. In fact the MgO could trap charges when it contains dislocations but in our numerical model the material was supposed to be perfect crystal (Figure 1). The trapping process, is easy after heating at 1000°C and 1500°C. For the second lattice (the Al₂O₃) the situation is different even after a small movement of the particle test, its localization is easy and confirms the ability of trapping charges for sapphire (Al₂O₃).

Figure 1 and figure 2 are the illustration of the trapping simulation. We have first run the simulation from a perfect crystal for 10,000 time steps (equal to 1ps) to be sure that the equilibration is reached; and it is done in the canonical form. The fluctuation of the cohesion energy of the crystal is controlled in an isothermal approach. Secondly an excess particle, is then introduced in the lattice. It movement is followed and the mean square displacement plotted as a function of the time, which inquire us on the ability of diffusion. The obtained results shown lead to Figure 1 and Figure 2.

4. Conclusion

The simulation is a powerful tool to study these phenomena. According to our first results, the numerical model studying trapping charge will be accurate through analytical studies by using the model based on quantum studies. Crystallographic
direction or dislocations have to be taken into account for our next studies.

References