Calculation of the spatial distribution of photovoltaic field by arbitrary 2D illumination patterns in $LiNbO_3$. Application to photovoltaic particle trapping.

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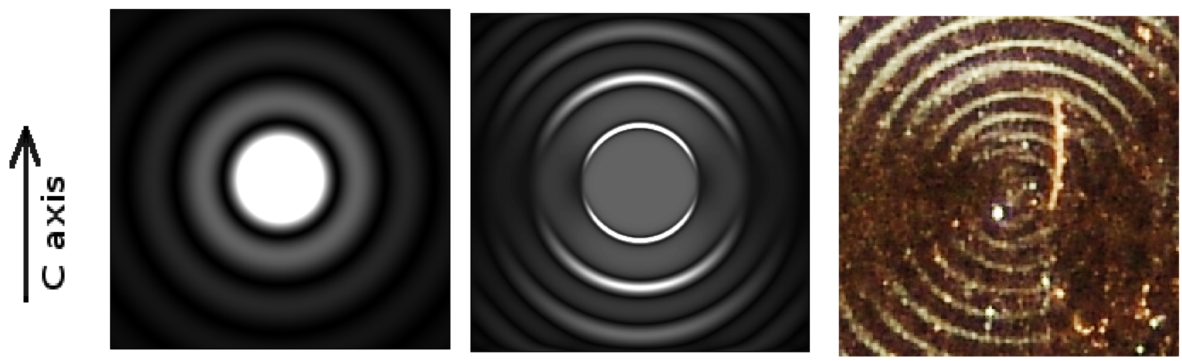
Summary

Patterns of evanescent photovoltaic field induced by illumination on a surface of lithium niobate (LN) have been calculated and compared with the experimental patterns of nano- and microparticles trapped by dielectrophoretic forces. A tool for this calculation has been developed.

Discussion

Photovoltaic tweezers are a promising tool to arrange and move particles on surfaces. The spatial distribution of electric field on photovoltaic materials as $Fe{:}LiNbO_3$ is a well known issue when illumination follows some analytical patterns, as low modulation sinusoidal pattern obtained by the interference of planar waves [1,2]. For a general illumination pattern, a numerical tool is needed to evaluate the electric field distribution that gives rise to the particle trapping pattern via electrophoretic or dielectrophoretic forces.

The calculation of the electric field pattern is based on the standard single centre model for charge-transport in LN [1,2]. The calculation consists in a time resolution of Kukhtarev equations for charge distribution, in an illuminated surface, by a finite differences algorithm. As a representative example, we show in figure 1 the results for a crystal illumination with an Airy disc distribution: (a,b) show the light intensity pattern (saturated on the center to see the low intensity oscillations) and the calculated electric field distribution, (c) shows the experimental trapping of micrometric chalk powder on a LN surface. *c*-axis is contained in the surface. Despite the actual light intensity profile is not well known for the experiment and the different scales, there is a good concordance: in the stable charge distribution, a set of ring sectors of electric field appears in between the light rings. These sectors have a crescent shape, with the maximum along the crystal *c*-axis. The trapped particle distribution in experiment follows the same pattern.



(a) (b) (c)

Fig. 1. Results for an Airy disc illumination of the $LiNbO_3$ surface: (a) light intensity pattern, (b) calculated electric field, (c) particle pattern obtained using $CaCO_3$ particles after illumination through a pin hole.

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References

[1] F. Agulló-López, G.F. Calvo, and M. Carrascosa, “Fundamentals of Photorefractive Phenomena” in *Photorefractive Materials and Applications 1*, P. Günter and J-P. Huignard Eds. (Springer, New York 2006) Chap 3, 2006

[2] Javier Villarroel, Hector Burgos, Angel García-Cabañes, Mercedes Carrascosa, Alfonso Blázquez-Castro, and Fernando Agulló-López, “Photovoltaic versus optical tweezers”, *Optics Express.* **19**(24) 24320, 2011

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Summary

Patterns of evanescent photovoltaic field induced by illumination on a surface of lithium niobate have been calculated and compared with the experimental patterns of nano- and micro particles trapped by dielectrophoretic forces.

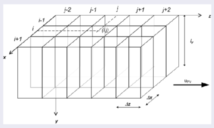
A tool for these calculations has been developed.

Model

Kukhtarev equations

$$\frac{\partial n}{\partial t} = sIN_D - \gamma n N_A - \frac{1}{q}\nabla\cdot\vec{J}$$
$$\frac{\partial N_D}{\partial t} = -\frac{\partial N_A}{\partial t} = -sIN_D + \gamma n N_A$$
$$\vec{J} = q\mu n\vec{E} - qD\vec{\nabla}n + qsIN_D L_{PV}\vec{u}_{PV}$$

Finite differences

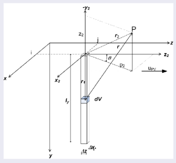


Internal electric field:

$$\vec{E}^t_{i,j} = \frac{ql_y\triangle x\triangle z}{4\pi\varepsilon_o}\sum_a\sum_b\frac{n_{a,b}+\triangle N_D^{a,b}}{\left(\sqrt{(\triangle z)^2(j-b)^2+(\triangle x)^2(i-a)^2}\right)^3}\left[\frac{\triangle z\,(j-b)}{\varepsilon_{a,b}}\vec{k}+\frac{\triangle x\,(i-a)}{\varepsilon_{a,b}}\vec{i}\right]$$

External electric field

calculation



Extension

- Hundred μm above the crystal
- Appropriate boundary and periodical conditions

Model

Calculus

Adiabatic Approximation

$$\frac{\partial n}{\partial t} = sIN_D - \gamma n N_A - \frac{1}{q}\vec{\nabla}\cdot\left[q\mu n\vec{E} - qD\vec{\nabla}n + qsIN_D L_{PV}\vec{u}_{PV}\right] \sim 0 \qquad \left(\ll \frac{\partial N_D}{\partial t}, \frac{\partial N_A}{\partial t}\right)$$

Finite differences

$$n^t_{k-NJ-2}(A_x+C_x) + n^t_{k-1}(C_y+A_y) + n^t_k(-G-D_{xy}-2A_x-2A_y) + \\ +n^t_{k+1}(A_y-C_y) \; +n^t_{k+NJ+2}(A_x-C_x) = F_x$$

where:

$$\begin{aligned} A_x &= cte \\ A_y &= cte \\ D^t_{xy} &= D^t_{xy}(E^t_x, E^t_y) \\ D^t_{xy} &= D^t_{xy}(E^t_x, E^t_y) \\ F^t_x &= F^t_x(I^t, N^t_D) \\ G^t &= G^t(N^t_D) \end{aligned}$$

- $\overline{\overline{K}}\vec{n} = \vec{B} \Longrightarrow \vec{n} = \overline{\overline{K}}^{-1}\vec{B}$

Crank-Nicolson

$$N_{D}{}^{t+1}_{i,j} = \frac{N_{D}{}^t_{i,j}\left[1-\alpha_d\triangle t\left(sI_{i,j}+\gamma n^t_{i,j}\right)\right]+\triangle t\gamma n^t_{i,j}N}{1+(1-\alpha_d)\triangle t\left(sI_{i,j}+\gamma n^t_{i,j}\right)}$$

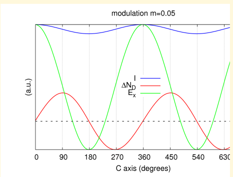
- Unconditionally stable with $\alpha_d \geq 0.5$
- $\triangle t < \frac{1}{\alpha_d(\gamma n^t_{i,j}+sI_{i,j})}$

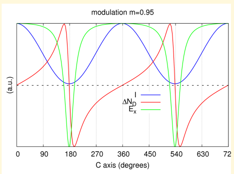
Convergence and control

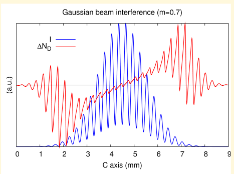
- Current divergence: $\max(\vec{\nabla}\cdot\vec{J_{i,j}}) \to 0$
- Residual: $\vec{r^l} = \vec{B^l} - K^l\vec{v^l} = Kv^{\vec{l+1}} - K\vec{v^l} = K\vec{e} \to 0$
- Charge neutrality: $\triangle x\triangle y\triangle z\sum_{a=1}^{NI}\sum_{b=1}^{NJ}\left(n_{a,b}+\triangle N_D^{a,b}\right) = 0$

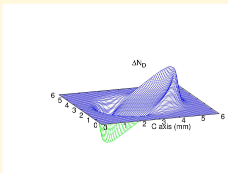
Calculations

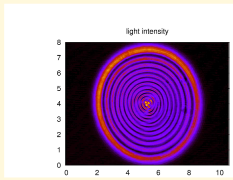
Internal



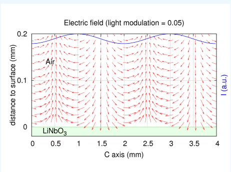


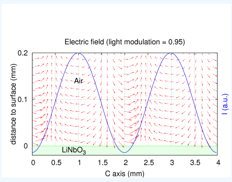


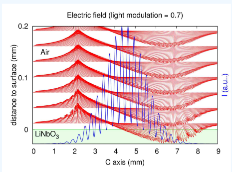


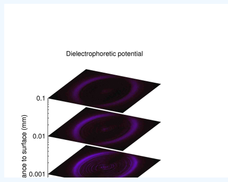


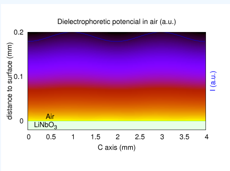
External

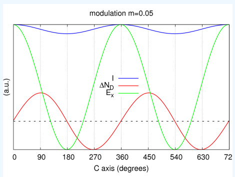


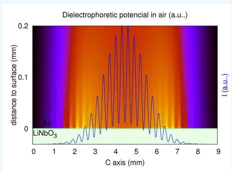


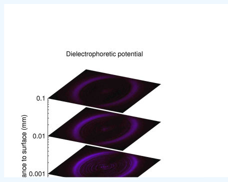




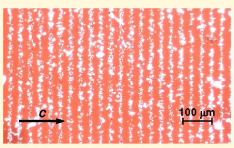


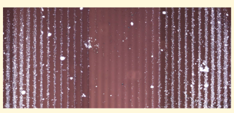


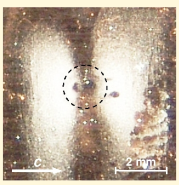


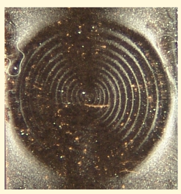


Experimental trapping









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