Fallo mecánico debido a grietas en Niobato de Litio bajo irradiación, simulación mediante elementos finitos

David Garoz, Antonio Rivera (IFN-UPM)
Fernando Agulló, José Olivares, M. Crespillo (CMAM)
Index

- Ion-induced nano-track in LiNbO3
- Motivation. From macro to nanoscale
- Finite element method for nano-structured materials
- Simulations of X-cut and Z-cut in LiNbO3
- Experiments versus Simulations
- Conclusions
Ion-induced nano-tracks in LiNbO₃

Swift heavy ions exceeding MeV/amu produce columnar nano-tracks around the straight ion trajectory, with marked modifications with respect to the virgin material.

High fluence induces cracks (macroscopic effect)

Crespillo et al. 2011
Rivera et al. 2011
From macro to nano-scale

Time

- Years
- Hours
- Minutes
- Seconds
- Microseconds
- Nanoseconds
- Picoseconds
- Femtoseconds

Distance

- 1A
- 1nm
- 1µm
- 1mm
- meters

Experiments

Material Properties

Mesoscale modeling, MC

Quantum mechanics (MD)

Continuum modes, Solid Mechanics (FEM)

Thermo-mechanical response

http://www.kintechlab.com/solutions/methodology/
- Deposited energy heat the nano-track over fusion temperature
- The cooling left an amorphous nano-track with lower density
- The dilatation of nano-track induce deformations and stresses
- A hillock per nano-track are expected at surface

6 nm radius nano-track with stress in Y direction.
Finite element method for nano-structured materials

- Geometry simple but with huge range scales
- Orthotropic properties in crystal LiNbO₃, and isotropic properties in amorphous track
- Boundary condition to simulate single track or multiple track (high fluence)
Simulations of X-cut in LiNbO₃

Hillcock has an elliptic shape due to orthotropic properties.

Simulations agree with analytical solution Colin et al. 2009.
Experiments versus simulations

Experimental values of hillcocks are over the simulation ones.

X-cut swelling simulations agree with experimental data at low fluences.
Cracks in X-cut

Cracks for fluence > 2 \times 10^{11}

Preference direction ±45°
Finite elements can be used in nano-scale to fill the gap between theory and experiments.

The elastic model must be complemented with plasticization to complete the ion-induce nano-tracks problem.
Thank you

Gracias