Crack mechanical failure in ceramic materials under ion irradiation: case of lithium niobate crystal

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• Experimental studies of nano-track in LiNbO₃
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Ion-induce nano-track

- Swift heavy ions produce amorphous tracks in many materials
- Mechanism dominated by electronic-excitation effects
- Marked threshold
- Final nanostructure with hillock formation

Ion track evolution
Schiwietz 2004
Lithium Niobate

- Important optical material
- Anisotropic crystal
- Symmetry C₃
- X-cut: anisotropic
- Z-cut: almost isotropic

Crystallographic structure LiNbO₃
Rivera 2011

David Garoz 13/09/2012

TNT2012, Madrid (Spain)
Ion-induced nano-tracks in LiNbO$_3$

**Amorphous tracks**
- Radius = 2.5 nm
- Depth > 1 μm
- Hillock dx ≈ 3.5 nm
- Ellipsoidal shape in X-cut (anisotropic crystal)

Br 45 MeV on LiNbO$_3$

Pb 2.3 GeV on LiNbO$_3$

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Ion-induced nano-tracks in LiNbO$_3$

- Track overlapping leads to continuous layers and swelling
- Important effects
  - Waveguides

Rivera et al. PSSA 206 (2009) 1109

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Ion-induced nano-tracks in LiNbO$_3$

- Track overlapping leads to continuous layers and swelling
- Important effects
  - Cracks (Xe 11 MeV/amu)
  - X-cut cracks oriented along 45°
  - Z-cut cracks not oriented

Motivations

Complete the gap between the experimental results and theory with simulation.

Avoid mechanical failure of ceramic under ion irradiation studying numerically the mechanical behavior.
Finite elements for nano-tracks

- Geometry simple but with a **huge range of scales**
- **Orthotropic properties** in crystal LiNbO$_3$, and isotropic properties in amorphous track
- Boundary condition to **simulate single track or multiple tracks** (high fluence)
Finite elements for nano-tracks

- Amorphous tracks have **lower density** than the crystal
- We insert a **realistic cylindrical track**
- **Dilatation** induces deformations and stresses
- A hillock per nano-track are expected at surface

6 nm radius nano-track with stress in Y direction.
Exp. vs simulations: hillock

Although simulations agree with analytical solutions, they are below experimental values. Elastic effects do not account for phase transformation.
Exp. vs simulations: swelling

X-cut swelling simulations agree with experiments, at high fluence underestimate, because layer growth not considered.
Simulation X-cut: Stress

Maximum stress increases with fluence

19.4 GPa

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X-cut: Angle of maximum stress

Preference direction ±45°
Corresponding to the direction of maximum stresses
FEM allow us to give yield strength
Surface cracks

In progress full simulation of crack growth using X-FEM
Conclusions

- The detailed structure of ion-induced nano-tracks in LiNbO₃ has been studied.
- Theoretical simulations with finite elements have been used to describe mechanical behavior of nano-tracks.
- Initial study of crack grown with X-FEM to avoid mechanical failure.
Thanks for your attention
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