Crack mechanical failure in lithium niobate crystal under ion irradiation; novel simulation by extended finite elements.

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Electronic excitation effects

- Swift heavy ions produce amorphous tracks in many materials
- Mechanism dominated by electronic-excitation effects
- Marked threshold
- Hillock formation

Lithium Niobate

- Important optical material
- Anisotropic crystal
- Symmetry $C_3$
- Cut X: anisotropic
- Cut Z: almost isotropic

Ion-induced nano-tracks in LiNbO$_3$

TEM: Amorphous tracks

Br 45 MeV on LiNbO$_3$
R=2.5 nm

Ion-induced nano-tracks in LiNbO₃

AFM: Hillocks

Pb 2.3 GeV on LiNbO₃
dx ≈ 3.5 nm

AFM: Pores (after HF etch)
Elipsoidal shape (Cut X)

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
Track overlapping leads to continuous layers and swelling

Important effects

Xe 11 MeV/amu: cracks

Cut X oriented along 45°

Cut Z not oriented

Ion-induced nano-tracks in LiNbO₃

- Amorphization beyond threshold
- Hillock and pore formation
- Anisotropy in Cut X
- Overlapping leads to continuous layers and swelling
- Cracks observed, in Cut X they are oriented
From macro to nano-scale

- Experiments
- Material Properties
- Continuum modes, Solid Mechanics (FEM)
- Engineering design, Unit process design
- Mesoscale modeling, MC
- Molecular dynamics (MD)
- Quantum mechanics (QC)

Distance: 1Å, 1nm, 1µm, 1mm, meters

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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.
Finite element method for nano-structured materials

- Geometry simple but with a huge range of scales
- Orthotropic properties in crystal LiNbO3, and isotropic properties in amorphous track
- Boundary condition to simulate single track or multiple track (high fluence)
The hillock has an elliptic shape due to orthotropic properties of LiNbO$_3$.
Simulations of X-cut in LiNbO$_3$

Simulations agree with analytical solution of Colin et al. Phyl. Mag. A 81 (2001) 857...
Experiments versus simulations

Simulation are below experimental values. Elastic effects do not account for phase transformation.
• Simple models cannot simulate the process of track overlapping.
• X-cut swelling simulations agree with experiments, at high fluence underestimate.
• Because layer growth not considered.
• Tracks considered cylindrical.
Single track Br 45 MeV of 2.3 nm radius

Maximum stress (12 Gpa) at the top surface expressed with Von Mises stress.

Maximum stress (9 Gpa) at the bottom of the sample expressed with Von Mises stress.
For 45 MeV of incident radius
Cracks in X-cut

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

- Finite elements can be used in nano-scale to fill the gap between theory and experiments.
- The elastic model accounts for anisotropy in Cut X.
- The elastic model can not account for the hillock height due to phase transition.
- On the other hand, it explains well the results of swelling, except at high fluence probably due to extra growth of layer.
- Maximum stresses at track boundary over planes forming 45°.
- In progress full simulation of crack growth from seed in region of maximum stress.
- In progress MD and FE studies in quartz.
From macro to nano-scale

- Experiments
- Material Properties
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- Quantum mechanics (QC)

Distance:
- 1 Å
- 1 nm
- 1 μm
- 1 mm
- meters

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

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Thanks for your attention