THE EFFECT OF SWIFT HEAVY ION IRRADIATION ON THE MICROSTRUCTURES OF YAP, YAG AND YIG

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Materials & Methods

**Fission Fragments**
- Simulate
- Swift Heavy Ions
- Why?
- Similar Masses & Energies
- Advantage
- No Activation/Radioactivity

**Latent Tracks**
- Affected?
- Temperature & Electronic Energy Loss
- How?
- Morphology & Diameter

**SHIs**
- Ion energy (log scale)
- Electronic stopping
- Nuclear stopping
- Stopping power (log scale)
- latent tracks affected?
- SHIs

[Figure: Sphor (1998)]

**Why?**
- Advantage

**No Activation/ Radioactivity**
- Why?
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**Morphology & Diameter**
- How?
- Temperature & Electronic Energy Loss

**Swift Heavy Ions**
- Why?
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**Advantage**
- No Activation/Radioactivity

**Fission Fragments**
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**Electronic Energy Loss**
- How?

**Temperature & Electronic Energy Loss**
- How?

**Morphology & Diameter**
- How?
Materials & Methods

Time evolution of the interaction of swift heavy ion a solid.

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The initial interaction excites the electronic sub-system on a femtosecond time scale, whilst atomic motion and the creation of disorder occur on a picosecond time scale.
Outline

Part 1
YAP & YAG – Effects of Stopping Power & Temperature on Track formation.

Part 2
Low & High Velocity Ions in YIG.
Combined Results: YAP, YAG & YIG.

General Conclusions
The influence of stopping power and temperature on latent track formation in YAP and YAG

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Diameter vs. $S_e$ - YAP

$S_e \approx 13.1$ keV.nm$^{-1}$  $S_e \approx 18.4$ keV.nm$^{-1}$  $S_e \approx 26.3$ keV.nm$^{-1}$  $S_e \approx 45.1$ keV.nm$^{-1}$

167 MeV Xe / 9.5 µm  167 MeV Xe / 6 µm  167 MeV Xe  930 MeV Bi
Diameter vs. $S_e$ - YAG

$S_e \approx 13.1 \text{ keV.nm}^{-1}$

$S_e \approx 18.3 \text{ keV.nm}^{-1}$

$S_e \approx 23.4 \text{ keV.nm}^{-1}$

$S_e \approx 40.1 \text{ keV.nm}^{-1}$

167 MeV Xe / 9.5 µm

167 MeV Xe / 6 µm

167 MeV Xe

930 MeV Bi
YAG - ITS vs Experiment

Two curves are for the minimum \( (E_{\text{min}} = 0.24 \text{ MeV/u}) \) and maximum \( (E_{\text{max}} = 4.7 \text{ MeV/u}) \) ion energies.

The x-axis error is the variation in the stopping power as a result of the sample thickness.
Track diameters as a function of stopping power.

Solid lines correspond to the where a “molten” phase ($E_m=0.65$ eV/at) is assumed and dashed lines where a “boiling” phase ($E_v=1.37$ eV/at) is assumed.

Two curves; for the minimum ($E_{min}=0.24$ MeV/u) and maximum ($E_{max}=4.2$ MeV/u) ion energies are shown for the molten- and boiling-phase scenarios.

The x-axis error is the variation in the stopping power as a result of the sample thickness.
YAP & YAG - Diameter vs. Temperature

YAG - 107 MeV Kr

LNT

ABF

[101]

HAADF

700 °C

YAP - 220 MeV Xe

LNT

[001]

ABF

HAADF

700 °C

\[ K_{\text{YAG}}(T) = \frac{39}{T} \]
\[ K_{\text{YAP}}(T) = 2.10094 + \frac{1379.44793}{T} \]

Track diameters in both YAP and YAG as a function of temperature with a fixed stopping power.

Calculated values from the iTS model are also shown; the solid lines corresponding to calculations where a “molten” phase ($E_m=0.74$ eV/at for YAG; $E_m=0.65$ eV/at for YAP) is assumed and the dashed line where a “boiling” phase ($E_v=1.37$ eV/ at for YAP) is assumed.
Amorphous latent ion tracks form both YAP and YAG at $S_e > 11$ keV/nm. Track diameters increase with increasing stopping power.

Tracks in YAP are smaller than YAG at similar stopping powers. Approximately 10 keV/nm more energy required to produce tracks, in YAP, similar in size to YAG.

Thermal conductivity effects tracks sizes in these two materials. However complexity of the crystal structure also plays a role. YAG has a more complex unit cell and presents larger tracks, whereas YAP with a much simpler unit cell presents significantly smaller tracks.

Track size is best defined as a region where the average energy per atom is higher than energy necessary to induce a “molten” phase in YAG.

A better fit is achieved for YAP if the track size is defined as region where the average energy per atom is higher than energy necessary to induce a “boiling” phase in YAP.
Latent tracks in bulk yttrium-iron garnet crystals irradiated with low and high velocity krypton and xenon ions

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SHIs in YIG – Formation Efficiency

Efficiency of amorphous latent track formation as a function of electronic stopping power.

Black points represent experimental values from HAADF STEM imaging. Dashed line shows an exponential trend of efficiency with electronic stopping power just to guide eyes.
Amorphous latent track radii distributions for bulk YIG crystals irradiated at approximately the same $S_e$ value $\sim 16$ keV/nm for 0.4 MeV/u Xe (red) and 1.07 MeV/u Kr (green) and $S_e \sim 15$ keV/nm for 7 MeV/u Kr (blue).

Average radius of amorphous track decreases with the increase of ion velocity, which is in agreement with previously reported velocity effect [1].

The radii of amorphous tracks in bulk YIG are consistent with previously reported results from indirect techniques for $S_e > 13$ keV/nm where the efficiency of track formation is close to 100% and continuous cylindrical amorphous tracks are formed.

For $S_e < 13$ keV/nm an underestimation of track size by indirect methods is observed compared to direct methods, because the efficiency of track formation decreases, and discontinuous tracks are formed.

Almost no difference is observed for track sizes in bulk and pre-thinned samples analysed by TEM, which suggest an insignificant influence of sample thickness on track size YIG.

Definite indication of the Velocity Effect in YIG.
YAP, YAG and YIG
Diameter vs *Stopping Power*

Diameter vs Stopping Power

- YAG
- YAP
- YIG High V
- YIG Low V

Track Diameter (nm) vs Stopping Power (keV/nm)
YAP, YAG and YIG
Diameter vs. Temperature

Track Diameter vs Temperature (YIG)

- YAG (Se = 15.5 keV/nm)
- YAP (Se = 27 keV/nm)
- YIG (Se = 25.9 keV/nm)
General Conclusions

The Formation of Latent Ion Tracks in YAP, YAG and YIG are influenced by:

1. Thermal Conductivity
2. Ion Velocity
3. Stopping Power
4. Crystal Complexity

In order to create a more accurate model for the prediction of track formation we need a better understanding of the material properties which have been shown to play a role in track formation.
Recrystallization as the governing mechanism of ion track formation.

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Crystal Complexity & Track Formation

Radial electron density (left panel) and energy density (right panel) in MgO (filled circles), Al$_2$O$_3$ (solid lines) and YAG (open symbols) at different times after 167 MeV Xe ion passage. Color coding indicates different time instants.

Radial distribution of the excess lattice energy density around the trajectories of 167 MeV Xe in MgO, Al$_2$O$_3$ and YAG.
Snapshots of modeled 167 MeV Xe tracks in three materials at 100 fs after ion passage with the experimental latent tracks as insets. The scales of MD images and TEM insets are the same.
Snapshots of MD supercell (left panels) and simulated X-ray powder diffraction patterns (right panels) of MgO, Al₂O₃ and YAG at different times after the passage of 167 MeV Xe ion.
Crystal Complexity & Track Formation

Modelled radial distribution functions of MgO, Al₂O₃ and YAG in the virgin states (solid lines) and at 1 ps after 167 MeV Xe impact (dashed lines).
Crystal Complexity & Track Formation

Left panel, snapshots of MD cells of MgO, Al₂O₃ and YAG sublattices after passage of 167 MeV Xe ion. Time instances show the initial stage of track size reduction (recrystallization). Grey dots are oxygen, black dots are Mg (MgO) and Al (Al₂O₃, YAG), red dots are Y atoms.

Right panel shows evolution of damaged track diameters in oxygen and magnesium sublattices of MgO.
Response of dielectric crystals: MgO, Al$_2$O$_3$, and Y$_3$Al$_5$O$_{12}$ (YAG) to irradiation with 167 MeV Xe ions decelerating in the electronic stopping regime.

Notably different tracks in three oxides: MgO, Al$_2$O$_3$, and YAG irradiated with Xe (176 MeV). MC-MD hybrid code revealed: **Initial electronic excitations** in these materials is **similar**. Energy transferred from an excited electronic system to atoms is **nearly identical**. **Transient melting** in the three materials within the **same radius**.

However, the relaxation of the molten regions in the three targets is very different:

- **Nearly perfect recrystallization in MgO**
- **Partial recovery in Al$_2$O$_3$**
- **Almost no recovery is seen in YAG**

**Correlation between the lattice structure and track crystallization efficiency.**