The mechanisms of radiation damage of diamond

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Why try to model damage?

If we can understand the mechanisms, we can extrapolate from known particle damage to damage due to different particles and energies.

It is an interesting problem for a materials physicist, with many aspects.

Why diamond:

Because it had a reputation for being radiation-hard before any experiments had been done.

Now RD42 have many experimental results, but the understanding of the processes is at an early stage.

We are using intrinsic diamond, so no complications from dopant-radiation damage complexes.
The main mechanisms

- Neutral particles, charged particles, $\gamma$s,
- Knock-on atoms,
- Recombination,
- Annealing,
- Some questions
- and conclusions.
Neutral particles (neutrons)
Cross-section for nuclear processes negligible.
Major process is ballistic displacement of an atom.
Most neutrons pass straight through the diamond.
A collision forms a vacancy + knock-on atom.

Charged particles
Most of the particle’s energy is lost to ionisation and phonons (heat).
Displaces atoms by Rutherford scattering, producing vacancy + knock-on atom.
Knock-on atoms produce the most damage.
\( \gamma S \)

- Compton scattering dominates up to \( \sim 20 \) MeV, then pair production becomes significant.
- It is the scattered Compton electron, or the electron-positron pair, that do the damage.
- Very small cross-section for interaction.

**Knock-on atoms**

- Lose energy to ionisation and phonons.
- But cross-section for collisions is high - they displace many atoms - **the major cause of damage**.
- Easy to model using TRIM (or similar).
Recombination

• Most of the knock-on atoms are displaced by only a few Å.

• Do they migrate straight back to recombine with the vacancy?
  – it depends on the type of diamond,
  – and the temperature,
  – and even the type of radiation.

• A more complex problem than we anticipated!

• We study it by annealing irradiated diamond...
Annealing

The vacancy has an activation energy for migration of 2.3 eV - it’s immobile below ~ 850 K.

The interstitial has an activation energy for migration of 1.6 eV - immobile below ~ 600 K.

Therefore (much simpler than Si!):

if we irradiate at room temperature, there should be no recombination - not true!

If we irradiate above ~ 600 K, there should be no surviving primary damage - not true either!

If we irradiate above ~ 850 K, there should be no surviving primary damage - this is true!
The experiments

1. Irradiate cold (~100K), anneal, monitor V and I.
2. Irradiate at 100-900K, monitor V and I.
3. Irradiate different types of diamond with $e^-$ and $\gamma$, monitor V and I.
4. In above experiments, look at other optical and EPR defects, and their evolution.

(This is a very brief summary of many experiments, over ~10 years, by many different people.)

How can you monitor concentrations?

V, V\textsuperscript{-}, V\textsuperscript{+}, V\textsubscript{2}, I + various NV complexes by optical spectroscopy,
V\textsuperscript{-}, V\textsuperscript{0}(excited state), I, I\textsubscript{2}, + various NV complexes by EPR.
Quite reliable concentrations from intensities.
Anneal diamond irradiated cold

Interstitials disappear at ~ 600 K (migrate to traps).
Vacancies disappear at ~ 900 K (migrate to traps - mainly N).
Irradiate at different temperatures

Annealing stages at:

- 150 K and 500 K for I,
- 500 K and 800 K for V.
Irradiation - conclusions

At low T, $[V] = [I]$.  
At ~ 150K, ~20% V, but ~60% I disappear.  
Therefore:  
  20% I recombining with V, NOT the normal migration process.  
  40% I disappearing elsewhere.  

Similar annealing stages as before, but at slightly lower T.  
Lower T probably due to local heating at displacement site.  

Almost no V-I recombination when I become (normally) mobile.  
Most of the I are NOT recombining with V, nor forming EPR-active I$_2$ (called R1). Where are they going?  

V are forming V$_2$ or N-V complexes when V are mobile.
Irradiate different types of diamond

e\textsuperscript{-} - irradiation, natural: pure diamond (IIa), N-aggregates (Ia)

We find ~60\% more vacancies in diamonds with N aggregates
N aggregates suppress the V-I recombination.

\(\gamma\) - irradiation, single crystal:

Pure diamond (IIa): Low production of V, no I survive.
V-I recombination during irradiation.
N-containing (Ib): More vacancies (V\textsuperscript{-} + V\textsuperscript{0}), a few I, I-N complexes.
Very little V-I recombination, I trapped by N.

\(\gamma\) - irradiation, polycrystalline CVD:

~40\times as many V as in pure single crystals, ~half as many I as V.
[V] ~ as predicted by Compton scattering + e\textsuperscript{-} cross-section.
Strain completely suppresses V-I recombination. Some I may be trapped during irradiation in other defects or complexes.
Different diamonds - conclusions

The damage that survives is determined by the amount of recombination during irradiation:

- Pure single crystal diamond: most V and I recombine under irradiation.
- N-containing diamond: more damage survives because the N enhances the separation of I & V.
- B-containing diamond: +ve charge states, not yet quantifiable.
- CVD diamond: Virtually no recombination under irradiation. Therefore very high surviving damage.

**WARNING:** results on single crystal diamond cannot be transferred to CVD polycrystalline diamond!

Probably dependent on the individual CVD samples?
Some questions

What are the actual unknown processes?
How do these [V] and [I] affect detection?
Can we engineer more rad-hard diamond?
What about priming?
Are complex defects affecting detection?
Is it going to be worth designing rad-hard diamond detectors for LHC?
Conclusions

• Knock-on atoms do more damage than the primary particle.
• V and I are immobile at RT, after irradiation, but I may migrate during irradiation.
• Recombination between I and V is crucial in determining how much damage survives.
• Polycrystalline CVD diamond shows much greater surviving damage than single crystal diamond - results not transferable.
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