Quantifying Radiation Damage in MX

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Quantifying Radiation Damage

1. Why
2. How
3. Problems
4. Solutions
5. New Stuff
Quantifying Radiation Damage

1. Why
Weik et al. (2002). JSR 9, 342-6; TcAChE; 10 MGy/dataset; densities from datasets 1 and 10
Quantifying Radiation Damage

2. How
Behaviour of a selection of reflexions, after correction for general effects, with exposure.
Fig. 6. Bar chart showing the number of damaged residues for each crystal vs. absorbed dose. The dotted vertical line indicates the experimentally determined value of $D_{1/2}$. Note that there are no disulfide bridges in ferritin, and these are known to be the most susceptible bonds.
Dose = \frac{\text{absorbed energy}}{\text{mass}} \quad \left[ \text{Gy} = \frac{\text{J}}{\text{kg}} \right]
Garman limit
30 MGy, 0.7 $I_0$, measured

Henderson limit
20 MGy, 0.5 $I_0$, estimated
Quantifying Radiation Damage

3. Problems
Dose = \frac{\text{absorbed energy}}{\text{mass}}

\text{Gy} = \frac{\text{J}}{\text{kg}}
<table>
<thead>
<tr>
<th>Element</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na</td>
<td>19 M</td>
</tr>
<tr>
<td>Mg</td>
<td>12 M</td>
</tr>
<tr>
<td>P</td>
<td>4 M</td>
</tr>
<tr>
<td>S</td>
<td>3 M</td>
</tr>
<tr>
<td>Cl</td>
<td>2.5 M</td>
</tr>
<tr>
<td>K</td>
<td>1.6 M</td>
</tr>
<tr>
<td>Ca</td>
<td>1.3 M</td>
</tr>
<tr>
<td>Fe</td>
<td>560 mM</td>
</tr>
<tr>
<td>Cu</td>
<td>430 mM</td>
</tr>
<tr>
<td>Zn</td>
<td>400 mM</td>
</tr>
<tr>
<td>As</td>
<td>350 mM</td>
</tr>
<tr>
<td>Se</td>
<td>340 mM</td>
</tr>
<tr>
<td>Br</td>
<td>1.2 M</td>
</tr>
<tr>
<td>I</td>
<td>230 mM</td>
</tr>
<tr>
<td>Gd</td>
<td>110 mM</td>
</tr>
<tr>
<td>Ta</td>
<td>75 mM</td>
</tr>
<tr>
<td>Pt</td>
<td>100 mM</td>
</tr>
<tr>
<td>Au</td>
<td>100 mM</td>
</tr>
<tr>
<td>Hg</td>
<td>88 mM</td>
</tr>
<tr>
<td>U</td>
<td>100 mM</td>
</tr>
</tbody>
</table>

Table 1
Dose-doubling concentration at 12680 eV/0.9793 Å (the Se edge).

Table 2

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average Dose (Whole Crystal)</td>
<td>1.5 MGy</td>
</tr>
<tr>
<td>95% Threshold (1.11 MGy) Average Dose</td>
<td>6.0 MGy</td>
</tr>
<tr>
<td>Maximum Dose</td>
<td>30.3 MGy</td>
</tr>
<tr>
<td>Dose Contrast (Maximum/Threshold Average)</td>
<td>5.05</td>
</tr>
<tr>
<td>Total absorbed energy</td>
<td>1.86 mJ</td>
</tr>
<tr>
<td>Dose Inefficiency (Maximum Dose/Absorbed Energy)</td>
<td>$1.6 \times 10^4$ kg$^{-1}$</td>
</tr>
</tbody>
</table>
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4. Solutions
Figure 5
Flow chart showing the stages used by RADDPOSE to calculate the dose absorbed by a crystal. The steps involved in the fluorescence escape corrections are coloured blue. Initially the contribution of a given
Crystal
Type Cuboid
Dimensions 100 100 100  # Dimensions of the crystal in X,Y,Z in μm.
   # Z is the beam axis, Y the rotation axis and
   # X completes the right handed set
   # (vertical if starting face-on).

PixelsPerMicron 0.3
AbsCoefCalc RDV2  # Absorption Coefficients Calculated using
   # RADDOSE v2 (Paithankar et al. 2009)

UnitCell 78.02 78.02 78.02  # unit cell size. angles default to 90°
NumMonomers 24  # number of monomers in unit cell
NumResidues 51  # number of residues per monomer

ProteinHeavyAtoms Zn 2 S 6  # heavy atoms added to protein part of the
   # monomer, i.e. S, coordinated metals

SolventHeavyConc P 425  # concentration of elements in the solvent
   # in mmol/l. Oxygen and lighter elements
   # should not be specified

SolventFraction 0.64  # fraction of the unit cell occupied by solvent

Beam
Type Gaussian  # can be Gaussian or TopHat
Flux 1e12  # in photons per second (2e12 = 2 * 10^12)
FWHM 20 20  # in μm, vertical by horizontal for a Gaussian beam
Energy 12.1  # in keV

Collimation Rectangular 100 100  # Vertical/Horizontal collimation of the beam

Wedge 0 120  # Start and End rotational angle of the crystal
ExposureTime 600  # Total time for entire angular range
Crystal
Type Cuboid
Dimensions 100 100 100  # Dimensions of the cuboid
# Z is the beam axis
# X completes the (vertical if s

PixelsPerMicron 0.3
AbsCoefCalc RDV2  # Absorption Coefficient
# RADDOS v2 (Paiv
UnitCell 78.02 78.02 78.02  # unit cell
NumMonomers 24  # number of monomers
NumResidues 51  # number of monomers
ProteinHeavyAtoms Zn 2 S 6  # heavy atoms in monomer,
SolventHeavyCo
SolventFraction

Beam
Type Gaussian  # can be Gaussian
Flux 1e12  # in photons per
FWHM 20 20  # in μm, vertical
Energy 12.1  # in keV
Collimation Rectangular 100 100  # Vertical

Wedge 0 120  # Start and End
ExposureTime 600  # Total time for

1.5 Figure S5 – Observing the Experiment

Figure S5: UML class diagram. Classes that implement the output interface can subscribe to an Experiment by calling its addObserver() method. The Experiment class will inform all subscribed objects when a new Crystal or...
import se.raddo.radose3D;

package se.raddo.radose3D;

public class BeamFactory {

    /**
     * creates and returns different Beam type objects.
     *
     * @param beamName
     * the name of the beam class requested.
     * @param properties
     * a Map containing the complete list of beam properties. Each beam type may require a different set of specified properties, but flux and energy etc. will certainly be required. Keys of the Map structure are usually determined by the constants defined in @link Beam), but third party Beam implementations may have their own key set. Check the corresponding beam class for details.
     * @return
     * The newly created object should not keep any references to this Map after object creation.
     */
    public Beam createBeam(final String beamName,
                           final Map<Object, Object> properties) {

        // 1. Do some sanity checks on the passed parameters
        if (beamName == null) {
            throw new RuntimeException("BeamFactory: beamName set to null");
        }
        if (properties == null) {
            throw new RuntimeException("BeamFactory: properties set to null");
        }

        String trimmedBeamName = beamName.trim();
        if (trimmedBeamName.equals("")) {
            throw new BeanNameException("BeamFactory: beamName is empty");
        }

        // 2. Construct the class name of the requested beam type
        String beamClassName = trimmedBeamName.replace("-", "").replace("_", "");
        if (trimmedBeamName.indexOf(".") == -1) {
            beamClassName = "Beam";
        }

        try {
            Class<?> clazz = Class.forName("se.raddo.radose3D." + beamClassName);
            Constructor<?> constructor = clazz.getDeclaredConstructor();
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5. New Stuff
To fully use the time and space resolved description of the dose state provided by RADDose-3D, we propose a metric against which to quantify radiation damage: diffraction-weighted dose (DWD).

For an MX experiment, DWD is a function of the spatial distribution of the dose state and the exposure of the crystal over a short time step. Mathematically, we define the DWD for the angular range exposed between time $t_{i-1} \rightarrow t_i$ as

$$DWD = \frac{\int_{t_{i-1}}^{t_i} \int_{\text{crystal}} D(V, t)F(V, t)dVdt}{\int_{t_{i-1}}^{t_i} \int_{\text{crystal}} F(V, t)dVdt},$$

[1]
Thank you
Dose distribution and aggregate statistics:

RADDOSE-3D:

DWD: