Radiation defect data for a Virtual Tokamak Reactor model

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Integrated model for a tokamak reactor

Plasma as a 3D neutron source

Neutron spectra at various locations in a DEMO power plant

Transmutations

Defect production

Transmutations: fission vs fusion

Minima in the neutron spectra correspond to resonances in the neutron absorption cross-section. Neutron absorption gives rise to transmutations.

Note the enhanced low energy part of n-spectra in fission reactors.

M.R. Gilbert and J.-C. Sublet, Nuclear Fusion 51 (2011) 043005
Transmutations: fission vs fusion

**Fission**

- Time: 0.00 seconds
- Pure W irradiated in HFIR spectrum
- Total flux: $5.1 \times 10^{15}$ n cm$^{-2}$ s$^{-1}$
- m - concentration dominated by metastable nuclide(s)

<table>
<thead>
<tr>
<th>Z</th>
<th>108</th>
<th>109</th>
<th>110</th>
<th>111</th>
<th>112</th>
<th>113</th>
<th>114</th>
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<tbody>
<tr>
<td>N</td>
<td>Pure W irradiated in HFIR spectrum</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Fusion**

- Time: 0.00 seconds
- Pure W irradiated in a typical DEMO FW armour spectrum
- Total flux: $6.60 \times 10^{14}$ n cm$^{-2}$ s$^{-1}$
- m - concentration dominated by metastable nuclide(s)

**Water cooling problematic**

In situ transmission electron microscope observation of accumulation of radiation damage in pure tungsten, bombarded by 150 keV W+ ions at 30K.
Invisible effects of irradiation

Comparison of electron microscope images of microstructure of unirradiated and irradiated, at 290 degrees C, F2W steel.

Neutron irradiated to 0.2 dpa

Unirradiated

Data courtesy of G.R. Odette and J. Haley, UCSB and Oxford
Invisible effects of irradiation

X. Yi et al., EPL 110 (2015) 36001

Cu irradiated by 60 MeV Ni ions

X-ray diffraction

B.C. Larson, Crystals 9 (2019) 257

\[ F(N) = \frac{A}{N^S}; \quad S \approx 1.8 \]

poor or no visibility

simulations

large defect clusters

experiment
Strain from exposure to irradiation

FIG. 1. Cross-section SEM images of a 5.0-μm-wide trench in a thermally grown SiO₂ film (a) before irradiation, and after 4.0 MeV Xe irradiation by (b) $1.0 \times 10^{15}$, (c) $3.0 \times 10^{15}$, and (d) $1.0 \times 10^{16}$/cm². All images were taken with the same magnification. The ion beam is directed perpendicular to the surface.

Dimensional changes in the stainless steel nuclear reactor components exposed to the neutron dose of ~ 75 dpa.

E. Snoeks et al., Appl. Phys. Lett. 65 (1994) 2487

Courtesy of F. Garner (2006)
Strain from exposure to irradiation

Two possible modes of swelling:

- volume increase due to voids in the bulk and “redeposition” of atoms to the surface or grain boundaries.
- macroscopic strain due to local microscopic distortions from invisible atomic-scale defects.


FIG. 4. TEM micrographs of the 3000 appm He implanted pure W. The image was recorded at ~1 μm underfocus. No Fresnel contrast was observed in a through-focus series indicating no He bubbles are present.
Above: a simplified model of DEMO used in neutron transport calculations. Right: (a) neutron energy spectra as functions of depth at the equatorial position and (b) at various positions in the divertor region.

Power density deposited by neutrons varies rapidly as a function of distance from the first wall. Energy is mostly deposited in the first 30cm of the blanket away from the plasma.


Fig. 2. Distributions of the 14 MeV neutron flux along the slit between the blanket modules under the neutron wall loading of 1 MW m\(^{-2}\), the blanket thickness of 45 cm, the blanket composition of 80% SS and 20% water, the vacuum vessel thickness of 40 cm, and the vacuum vessel shield composition of 60% SS and 40% water.
Accurate predictive neutron transport calculations can now be performed using engineering design drawings as input.

<table>
<thead>
<tr>
<th>Reactor</th>
<th>Locations</th>
<th>Total flux (1/cm²/sec)</th>
<th>DPA/year (Eurofer)</th>
<th>He gas production (appm)</th>
<th>H gas production (appm)</th>
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<tr>
<td><strong>DEMO</strong></td>
<td>First Wall</td>
<td>3.79E+14</td>
<td>9.5</td>
<td>108.4</td>
<td>536.0</td>
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<td></td>
<td>blanket 1st layer</td>
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<td>8.6</td>
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<td>blanket 3rd layer</td>
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<td>4.10E+10</td>
<td>4.9E-4</td>
<td>0.01</td>
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<td><strong>ITER TBM</strong></td>
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<td>1.86E+13</td>
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<td>4.4</td>
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<td>0.1</td>
<td>0.6</td>
<td>2.8</td>
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<tr>
<td></td>
<td>back plate</td>
<td>1.14E+12</td>
<td>7.4E-3</td>
<td>0.1</td>
<td>0.1</td>
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<tr>
<td><strong>PWR</strong></td>
<td>core equivalent</td>
<td>1.64E+14</td>
<td>1.8</td>
<td>12.2</td>
<td>10.4</td>
</tr>
<tr>
<td></td>
<td>core barrel</td>
<td>3.54E+13</td>
<td>0.3</td>
<td>3.0</td>
<td>1.5</td>
</tr>
<tr>
<td></td>
<td>RPV average</td>
<td>3.50E+10</td>
<td>2.9E-4</td>
<td>9.6E-4</td>
<td>1.1E-3</td>
</tr>
</tbody>
</table>

Characteristic values of neutron flux, radiation damage and gas production at various locations in DEMO, ITER TBMs and PWR. ITER D-T model assumptions: 30000 deuterium-tritium shots, each lasting approximately 400s.

S. Zhang et al., presentation at ICFRM16, Beijing, October 21-25, 2013.
Computing stress and strain in reactor components due to exposure to irradiation
Lattice distortions in Fe near a self-interstitial atom defect. Lattice distortions in engineering are known as “strain”, related to “stress” (internal forces).
Elastic fields of defects

\[ u_i(r) = -P_{kl} \frac{\partial}{\partial x_l} G_{ik}(r - R) \]

\[ G_{ik}(r) = \frac{1}{16\pi \mu (1 - \nu) r} \left[ (3 - 4\nu) \delta_{ik} + \frac{x_i x_k}{r^2} \right] \]

\[ P_{ij} = -\int_{V_{cell}} \sigma_{ij} dV = - V_{cell} \bar{\sigma}_{ij} \]

Elements of the dipole tensor are almost always computed, as a by-product of almost any DFT or molecular statics simulation involving atomic relaxations.

Elastic fields of defects

\[ u_i(r) = -P_{kl} \frac{\partial}{\partial x_l} G_{ik}(r - R) \]

\[ G_{ik}(r) = \frac{1}{16\pi \mu (1 - \nu) r} \left[ (3 - 4\nu) \delta_{ik} + \frac{x_i x_k}{r^2} \right] \]

\[ P_{ij} = -\int_{V_{cell}} \sigma_{ij} dV = -V_{cell} \bar{\sigma}_{ij} \]

\[ P_{kl} = C_{klmn} \Omega_{mn} \]

**relaxation volume tensor**: the sum of its diagonal elements equals the relaxation volume (= “the volume”) of the defect
Volumes of defects: literature data

Theoretical values of the vacancy formation volume, \( V_v \), in units of atomic volume, \( \Omega \), and the experimental data.

2. Jacucci and Taylor [107].
3. Bauer et al. [108].
4. Harder and Bacon [101].
5. Ackland et al. [102].
6. Rosato et al. [104].
7. Experimental data [109–111].

<table>
<thead>
<tr>
<th>Metal</th>
<th>( V_v/\Omega )</th>
</tr>
</thead>
<tbody>
<tr>
<td>K</td>
<td>0.59–0.71(^a)</td>
</tr>
<tr>
<td>Na</td>
<td>0.25</td>
</tr>
<tr>
<td>Li</td>
<td>0.2–0.25</td>
</tr>
<tr>
<td>In</td>
<td>0.45</td>
</tr>
<tr>
<td>Sn</td>
<td>0.25</td>
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<tr>
<td>Cd</td>
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</tr>
<tr>
<td>Pb</td>
<td>0.4</td>
</tr>
<tr>
<td>Zn</td>
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</tr>
<tr>
<td>Al</td>
<td>0.65</td>
</tr>
<tr>
<td>Ag</td>
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<tr>
<td>Au</td>
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<tr>
<td>Cu</td>
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<td>Ni</td>
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<td>Pb</td>
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<tr>
<td>Pt</td>
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<tr>
<td>V</td>
<td>0.76</td>
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<tr>
<td>Cr</td>
<td>0.84</td>
</tr>
<tr>
<td>Ir</td>
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<tr>
<td>Rh</td>
<td>0.84</td>
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<tr>
<td>Nb</td>
<td>0.96</td>
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<tr>
<td>Mo</td>
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<td>Ta</td>
<td>0.83</td>
</tr>
<tr>
<td>W</td>
<td>0.68</td>
</tr>
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</table>


Note the large variability of data: relaxation volumes are very difficult to measure accurately.
Evaluation of dipole tensors and volumes of defects using DFT

A general expression for elastic energy

\[ E_D = \frac{1}{2} \int_V \sigma_{ij}(\mathbf{r}) \epsilon_{ij}(\mathbf{r}) dV. \]

In the presence of small external strain, the following Taylor expansion applies:

\[ E_D(\epsilon_{ij}^{ext}) = E_D(\epsilon_{ij}^{ext} = 0) + \left( \frac{\delta E_D}{\delta \epsilon_{ij}^{ext}} \right)_{\epsilon_{ij}^{ext}=0} \epsilon_{ij}^{ext} + \cdots \]

Energy of interaction between a defect and external strain

\[ E = -P_{ij} \epsilon_{ij}^{ext} \]

Hence the dipole tensor of a defect can be computed from the stress that it produces in a simulation cell (no volume relaxation)

\[ P_{ij} = -\left( \frac{\delta E_D}{\delta \epsilon_{ij}^{ext}} \right)_{\epsilon_{ij}^{ext}=0} = -\int_V \sigma_{ij}^D dV. \]
Evaluation of dipole tensors and volumes of defects using DFT

Equations required for a numerical evaluation of the relaxation volume of a defect

\[ E = -P_{ij} \varepsilon_{ij}^{ext} \]

\[ \Omega_{ij} = S_{ijkl} P_{kl}. \]

\[ S = C^{-1} \] is the elastic compliance tensor

\[ C_{ijkl} S_{klmn} = \frac{1}{2} (\delta_{im} \delta_{jn} + \delta_{in} \delta_{jm}) \]

\[ \Omega_{\text{rel}} = Tr \Omega_{ij} = \Omega_{11} + \Omega_{22} + \Omega_{33} \]
The universal character of defect structure in various bcc metals, apart from Fe, which stands out because of magnetism. In other bcc metals, including simple alkaline metals, the lowest energy SIA defect structure is a 111 crowdion.
It is hard to offer a simple reason why the structure of a SIA defect appears universal for all the bcc metals. In sodium (left), the charge deformation associated with the defect is almost non-directional, whereas in tungsten (right), the effects of directional $d$-bonding are evident.
The symmetry-broken structure of an SIA defect in Cr, Mo and W

The structure of a symmetry-broken 111 self-interstitial atom defect in Cr, Mo and W. On average, the defect still migrates one-dimensionally. But symmetry breaking is responsible for the complex low temperature resistivity recovery stages in Cr, Mo and W. There is no symmetry-breaking in V, Nb, Ta.

Elastic dipoles and relaxation volumes of defects: direct DFT calculations

|   | \( P_{11} \) | \( P_{22} \) | \( P_{33} \) | \( P_{12} \) | \( P_{23} \) | \( P_{31} \) | \( \Omega_{11} \) | \( \Omega_{22} \) | \( \Omega_{33} \) | \( \Omega_{12} \) | \( \Omega_{23} \) | \( \Omega_{31} \) | \( \Omega^{(1)} \) | \( \Omega^{(2)} \) | \( \Omega^{(3)} \) | \( \Omega_{\text{rel}} \) |
|---|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| (110)d | 25.832 | 21.143 | 21.150 | 0.000 | 5.122 | 0.000 | 9.777 | 4.294 | 4.302 | 0.000 | 3.819 | 0.000 | 9.777 | 0.475 | 8.122 | 1.620 |
| Tetra | 21.396 | 23.331 | 23.339 | 0.000 | 0.001 | 0.000 | 4.607 | 6.871 | 6.880 | 0.000 | 0.000 | 0.000 | 4.607 | 6.871 | 6.880 | 1.619 |
| (100)d | 32.284 | 22.931 | 22.937 | 0.000 | 0.000 | 0.000 | 14.316 | 3.378 | 3.385 | 0.000 | 0.000 | 0.000 | 14.316 | 3.378 | 3.385 | 1.858 |
| Octa | 23.273 | 23.273 | 31.302 | 0.000 | 0.000 | 0.000 | 3.869 | 3.869 | 13.258 | 0.000 | 0.000 | 0.000 | 3.869 | 3.869 | 13.258 | 1.851 |
| Vac | −3.081 | −3.081 | −3.081 | 0.000 | 0.000 | 0.000 | −0.831 | −0.831 | −0.831 | 0.000 | 0.000 | 0.000 | −0.831 | −0.831 | −0.831 | −0.220 |

|   | \( P_{11} \) | \( P_{22} \) | \( P_{33} \) | \( P_{12} \) | \( P_{23} \) | \( P_{31} \) | \( \Omega_{11} \) | \( \Omega_{22} \) | \( \Omega_{33} \) | \( \Omega_{12} \) | \( \Omega_{23} \) | \( \Omega_{31} \) | \( \Omega^{(1)} \) | \( \Omega^{(2)} \) | \( \Omega^{(3)} \) | \( \Omega_{\text{rel}} \) |
|---|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| (110)d | 56.960 | 52.557 | 52.557 | 0.000 | 11.277 | 0.000 | 10.908 | 8.693 | 8.693 | 0.000 | 6.358 | 0.000 | 10.908 | 2.335 | 15.050 | 1.753 |
| Tetra | 47.359 | 59.114 | 59.114 | 0.000 | 0.000 | 0.000 | 5.693 | 11.606 | 11.606 | 0.000 | 0.000 | 0.000 | 5.693 | 11.606 | 11.606 | 1.791 |
| (100)d | 65.920 | 53.379 | 53.379 | 0.000 | 0.000 | 0.000 | 14.254 | 7.945 | 7.945 | 0.000 | 0.000 | 0.000 | 14.254 | 7.945 | 7.945 | 1.868 |
| Octa | 52.741 | 52.741 | 67.209 | 0.000 | 0.000 | 0.000 | 7.623 | 7.623 | 14.901 | 0.000 | 0.000 | 0.000 | 7.623 | 7.623 | 14.901 | 1.868 |
| Vac | −9.984 | −9.984 | −9.984 | 0.000 | 0.000 | 0.000 | −1.743 | −1.743 | −1.743 | 0.000 | 0.000 | 0.000 | −1.743 | −1.743 | −1.743 | −0.324 |
# Elastic dipoles and relaxation volumes of defects: direct DFT calculations

## TABLE VI. Elements of the dipole tensor \( P_{ij} \) (in eV units), the relaxation volume tensor \( \Omega_{ij} \) (in Å³ units), eigenvalues of the relaxation volume tensor \( \Omega^{(i)} \) (in Å³ units), and the relaxation volume of the defect \( \Omega_{\text{rel}} \) (in atomic volume units \( \Omega_0 \)) computed for Li.

| Li   | \( P_{11} \) | \( P_{22} \) | \( P_{33} \) | \( P_{12} \) | \( P_{23} \) | \( P_{31} \) | \( \Omega_{11} \) | \( \Omega_{22} \) | \( \Omega_{33} \) | \( \Omega_{12} \) | \( \Omega_{23} \) | \( \Omega_{31} \) | \( \Omega^{(1)} \) | \( \Omega^{(2)} \) | \( \Omega^{(3)} \) | \( \Omega_{\text{rel}} \) |
|------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| (111)d | 2.071       | 2.071       | 2.071       | 0.796       | 0.796       | 0.796       | 7.930       | 7.930       | 5.577       | 5.577       | 5.577       | 2.353       | 2.353       | 19.084      | 1.175       |
| (111)c | 2.063       | 2.063       | 2.063       | 0.761       | 0.761       | 0.761       | 7.899       | 7.899       | 5.334       | 5.334       | 5.334       | 2.566       | 2.566       | 18.567      | 1.171       |
| (110)d | 2.109       | 2.188       | 2.188       | 0.000       | 0.727       | 0.000       | 6.936       | 8.947       | 0.000       | 5.096       | 0.000       | 6.936       | 3.851       | 14.043      | 1.227       |
| Tetra | 2.196       | 2.160       | 2.160       | 0.000       | 0.000       | 0.000       | 8.923       | 8.011       | 0.000       | 0.000       | 0.000       | 8.923       | 8.011       | 8.011       | 1.232       |
| (100)d | 2.764       | 1.911       | 1.911       | 0.000       | 0.000       | 0.000       | 22.893      | 1.164       | 0.000       | 0.000       | 0.000       | 22.893      | 1.164       | 1.164       | 1.246       |
| Octa | 1.898       | 1.898       | 2.754       | 0.000       | 0.000       | 0.000       | 1.094       | 1.094       | 22.892      | 0.000       | 0.000       | 1.094       | 1.094       | 22.892      | 1.239       |
| Vac | -0.937      | -0.937      | -0.937      | 0.000       | 0.000       | 0.000       | -3.589      | -3.589      | -3.589      | 0.000       | 0.000       | -3.589      | -3.589      | -3.589      | -0.532      |

## TABLE XVI. Elements of the dipole tensor \( P_{ij} \) (in eV units), the relaxation volume tensor \( \Omega_{ij} \) (in Å³ units), eigenvalues of the relaxation volume tensor \( \Omega^{(i)} \) (in Å³ units), and the relaxation volume of the defect \( \Omega_{\text{rel}} \) (in atomic volume units \( \Omega_0 \)) computed for Mo.

| Mo   | \( P_{11} \) | \( P_{22} \) | \( P_{33} \) | \( P_{12} \) | \( P_{23} \) | \( P_{31} \) | \( \Omega_{11} \) | \( \Omega_{22} \) | \( \Omega_{33} \) | \( \Omega_{12} \) | \( \Omega_{23} \) | \( \Omega_{31} \) | \( \Omega^{(1)} \) | \( \Omega^{(2)} \) | \( \Omega^{(3)} \) | \( \Omega_{\text{rel}} \) |
|------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| (110)d | 42.470      | 39.944      | 39.944      | 0.000       | 6.757       | 0.000       | 9.196       | 7.896       | 0.000       | 5.429       | 0.000       | 9.196       | 2.468       | 13.325      | 1.584       |
| Tetra | 37.531      | 43.685      | 43.685      | 0.000       | 0.000       | 0.000       | 6.391       | 9.558       | 9.558       | 0.000       | 0.000       | 6.391       | 9.558       | 9.558       | 1.617       |
| (100)d | 48.989      | 40.370      | 40.370      | 0.000       | 0.000       | 0.000       | 11.788      | 7.353       | 7.353       | 0.000       | 0.000       | 11.788      | 7.353       | 7.353       | 1.680       |
| Octa | 39.601      | 39.601      | 50.174      | 0.000       | 0.000       | 0.000       | 6.994       | 6.994       | 12.435      | 0.000       | 0.000       | 6.994       | 6.994       | 12.435      | 1.675       |
| Vac | -9.576      | -9.576      | -9.576      | 0.000       | 0.000       | 0.000       | -1.956      | -1.956      | -1.956      | 0.000       | 0.000       | -1.956      | -1.956      | -1.956      | -0.372      |
Effects of symmetry

Averaging over orientations of the defect produces a diagonal tensor

\[
\begin{pmatrix}
P_a & P_b & P_b \\
-P_b & P_a & -P_b \\
-P_b & -P_b & P_a
\end{pmatrix}
\begin{pmatrix}
P_a & -P_b & P_b \\
-P_b & P_a & -P_b \\
-P_b & -P_b & P_a
\end{pmatrix}
\begin{pmatrix}
P_a & P_b & -P_b \\
-P_b & P_a & -P_b \\
-P_b & -P_b & P_a
\end{pmatrix}
\begin{pmatrix}
P_a & -P_b & -P_b \\
-P_b & P_a & P_b \\
-P_b & P_b & P_a
\end{pmatrix}
\]

\[
\begin{pmatrix}
P_a & 0 & 0 \\
0 & P_a & 0 \\
0 & 0 & P_a
\end{pmatrix}
= P_a \delta_{ij}
\]
Strain field of defects

In applications, we are interested in the elastic field produced by many defects => self-averaging

\[ \langle \Omega_{mn} \rangle = \sum_{s=1}^{3} \Omega^{(s)} \langle e_{m}^{(s)} e_{n}^{(s)} \rangle \]

\[ \langle \Omega_{mn} \rangle = \frac{1}{3} \Omega_{\text{rel}} \delta_{mn} \]

Anisotropic crystallographic effects are not significant for large structural components, since grain orientations are random

\[ \eta_{i} = \frac{(r - R)_{i}}{|r - R|} \]

\[ \omega_{\text{rel}}(r) = \sum_{a} \Omega_{\text{rel}}^{(a)} \delta(r - R_{\alpha}) \]

\[ \omega(r) \text{ is the density of relaxation volumes of defects.} \]
Macroscopic stress from defects

\[ \epsilon_{ij}(r) = \frac{1}{4\pi} \frac{1 + \nu}{1 - \nu} \int \frac{\omega_{\text{rel}}(R)}{|r - R|^3} \left( \frac{1}{3} \delta_{ij} - \eta_i \eta_j \right) d^3R. \]

\[ \epsilon_{ij}(r) = -\frac{1}{12\pi} \frac{1 + \nu}{1 - \nu} \int \omega_{\text{rel}}(R) \frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{|r - R|} d^3R. \]

The above two equations for strain are fully equivalent. Now we evaluate stress

\[ \sigma_{ij}(r) = -\frac{\mu}{6\pi} \frac{1 + \nu}{1 - \nu} \int \omega_{\text{rel}}(R) \frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{|r - R|} d^3R \]

\[ -\frac{\mu}{12\pi} \left( \frac{1 + \nu}{1 - \nu} \right) \left( \frac{2\nu}{1 - 2\nu} \right) \delta_{ij} \]

\[ \times \sum_k \int \omega_{\text{rel}}(R) \frac{\partial^2}{\partial x_k^2} \frac{1}{|r - R|} d^3R, \]

The second term is the contribution from the (singular!) core of the defect:

\[ \sum_k \frac{\partial^2}{\partial x_k^2} \frac{1}{|r - R|} = \Delta \frac{1}{|r - R|} = -4\pi \delta(r - R) \]
Macroscopic stress from defects

\[ \sigma_{ij}(\mathbf{r}) = -\frac{\mu}{6\pi} \frac{1 + \nu}{1 - \nu} \int \omega_{\text{rel}}(\mathbf{R}) \frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{|\mathbf{r} - \mathbf{R}|} d^3\mathbf{R}. \]

\[ + \frac{\mu}{3} \left( \frac{1 + \nu}{1 - \nu} \right) \left( \frac{2\nu}{1 - 2\nu} \right) \delta_{ij} \omega_{\text{rel}}(\mathbf{r}). \]

The total stress field generated by a distribution of defects. The density of body forces equals

\[ f_i(\mathbf{r}) = -\frac{\partial \sigma_{ij}(\mathbf{r})}{\partial x_j} = \frac{2\mu}{3} \left( \frac{1 + \nu}{1 - \nu} \right) \frac{\partial}{\partial x_i} \omega_{\text{rel}}(\mathbf{r}) \]

\[ - \frac{\mu}{3} \left( \frac{1 + \nu}{1 - \nu} \right) \left( \frac{2\nu}{1 - 2\nu} \right) \frac{\partial}{\partial x_i} \omega_{\text{rel}}(\mathbf{r}). \]

\[ \frac{\partial}{\partial x_j} \sigma_{ij}(\mathbf{r}) + f_i(\mathbf{r}) = 0 \quad f_i(\mathbf{r}) = -B \frac{\partial}{\partial x_i} \omega_{\text{rel}}(\mathbf{r}) \]

where \( B = 2\mu(1 + \nu)/[3(1 - 2\nu)] \) is the bulk modulus
A full condition of equilibrium includes gravity, thermal expansion, and swelling due to defects.

\[
\frac{\partial \sigma_{ik}(r)}{\partial x_k} + \rho g_i - B \alpha \frac{\partial T}{\partial x_i} - B \frac{\partial}{\partial x_i} \omega_{rel}(r) = 0.
\]

Defects, as opposed to temperature, generate compressive or tensile strains: this agrees with DFT – vacancies give rise to lattice contraction.

W. Hertz et al., Phys. Letters 43A (1973) 289
Volumes of all the possible defects

Relaxation volumes of (left) self-interstitial and (right) vacancy defects. The smallest defects produce the largest stresses and deformations per defect. The dominant contribution to stress in irradiated reactor components is from the smallest dislocation loops. Voids produce almost no stress.

Stress field produced by a cascade event

Stress field produced by a cascade event

It is now possible to compute macroscopic stress and strain from trillions of such cascade events occurring at various locations in a reactor component.
A case study: stress in an irradiated spherical shell

A steel shell containing a volumetric neutron source.

Case study 1

*Figures showing relaxation volume density and stress as a function of radial coordinate.*
Summary

Modelling radiation effects in materials, used in combination with high resolution *ex- and in-situ* experimental techniques, is progressing, facilitating new opportunities in engineering design.

Direct “mechanistic” approach, involving both the incremental development of established models (advanced DFT, machine learning potential-based MD) and fundamentally new mathematical algorithms, delivers steadily improving predictions.

Simulations of cascade events, and databases of defect structures produced in such events – including radiation damage events in microstructurally complex materials – provides the information critically significant for the development of microstructurally complex materials for advanced nuclear applications.