Cu has been simulated under a variety of conditions using a molecular dynamics code:
- Static uncompressed.
- Static uniaxially compressed.
- Shock elastically compressed.

By taking a Fourier transform of the atom positions, and using models for Debye temperature, an x-ray diffraction image can be simulated, from which we can glean intensities [4].

Debye-Waller Effect
- The normalised intensity of a diffraction peak, \( I(T) \), is related to temperature by
  \[
  I(T) = e^{-2M} 
  \]
  where
  \[
  2M \propto |G|^{2} \frac{T}{\Theta^2} 
  \]
  and \( G \) is the reciprocal lattice vector of the peak, \( T \) is temperature, \( \Theta \) is Debye temperature [3].
- Debye temperature is constrained by theory well enough to provide a temperature estimate that varies little with model used:

<table>
<thead>
<tr>
<th>Model Type</th>
<th>Hydrostatic: Error in T</th>
<th>Static Uniaxial: Error in T</th>
<th>Shock (Up = 0.5 km/s): Error in T</th>
</tr>
</thead>
<tbody>
<tr>
<td>Very Simple</td>
<td>+ 0.1 %</td>
<td>+ 5.7 %</td>
<td>+ 15.7 %</td>
</tr>
<tr>
<td>Perturbation theory</td>
<td>+ 0.1 %</td>
<td>+ 4.7 %</td>
<td>+ 14.3 %</td>
</tr>
<tr>
<td>Empirical</td>
<td>+ 0.1 %</td>
<td>+ 5.7 %</td>
<td>+ 15.7 %</td>
</tr>
<tr>
<td>Empirical + EOS</td>
<td>+ 0.1 %</td>
<td>+ 6.0 %</td>
<td>+ 16.0 %</td>
</tr>
</tbody>
</table>

Dislocations and Polycrystals
- Wilkins’ [5] line profile analysis techniques suggest that dislocations have little effect on the integrated diffraction intensity; simulations confirming this have yet to be completed.
- Polycrystals are not expected to interfere with the technique.
- A large simulation, with multiple grains, should be plastically shocked. This simulation will act as the closest approximation to experiment.

Future Work
- X-ray backlighter will be either Cu or Fe.
- Sample will be Nb.
- Scattered x-rays are collected on image packs which are placed in a geometry optimised for this experiment.
- This geometry allows for collection of photons from many locations around the diffraction rings.

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