Chapter 7

High strain deformation of single crystal copper: Experiments and MD simulations

As mentioned in Chapter 1, hydrodynamic simulations require three main inputs to simulate impact and shock wave problems:

- Fracture parameters.
- Material strength during high strain-rate deformation.
- Equation of state.

All previous chapters have dealt with fracture. In this chapter, material strength parameters for single-crystal copper have been obtained by performing experiments at $10^3$/s strain rate, using the Split Hopkinson Pressure Bar (SHPB) method [97].

Several workers [98–100] have performed experiments on single crystal copper to study the various aspects, such as activation of slip systems, under quasi-static loading. Here single crystal copper is uniaxially deformed at $10^3$/s strain rate to get material strength parameters.
7.1 Split Hopkinson Pressure Bar

7.1.1 Theory

An SHPB consists of a compressed gas-gun, a striker bar, pressure bars (incident and transmission bars), specimen and data acquisition system, as shown in Figure 7.1. To record the incident, reflected and transmitted waves, strain gauges are mounted on the incident and transmission bars. The striker bar, accelerated by gas, hits the incident bar, producing compressive stress waves at the point of impact. These waves move toward the free surfaces of the striker bar and the other end of the incident bar attached to the specimen. When the compressive wave reaches the free surface of the striker bar, it reflects as a tension wave. When this tension wave reaches the striker bar-incident bar interface, the striker bar gets separated out since tension can not pass through the interface. This leads to the creation of a compressive wave in the incident bar having a wave length (spatial duration) equal to twice the length of the striker bar. When the compressive wave reaches the incident bar-specimen interface, impedance mismatch occurs at the interface, leading to partial reflection of the wave as a tension wave in the incident bar and partial transmission of the compressive wave into the specimen. When the compressive wave reaches the specimen-transmission bar interface, again due to impedance mismatch, the wave is partially reflected as a compressive wave and partially transmitted as a compressive wave to the transmission bar. During this process, a compressive wave is trapped in the specimen which, by multiple reverberations, leads to plastic deformation of the specimen.

Using one-dimensional elastic wave propagation theory [101], assuming homogeneous deformation of the specimen under uniaxial stress conditions, the average...
or engineering strain, stress and strain-rate in the specimen are given by

\[
e_s(t) = -2 \frac{c_0}{l} \int_0^t \epsilon_R(t) dt \\
\sigma_s(t) = \frac{A}{A_s} \epsilon_T(t) \\
\dot{\epsilon}_s(t) = -2 \frac{c_0}{l} \epsilon_R(t)
\]  

(7.1) \hspace{1cm} (7.2) \hspace{1cm} (7.3)

where \( l \) is the initial length of the specimen, \( c_0 \) is the elastic wave velocity in the pressure bars (\( c_0 = \sqrt{E/\rho} \)), \( A \) is the cross-sectional area of the bar and \( A_s \) is the cross-sectional area of the specimen, \( E \) is the Young’s modulus of the bar, \( t \) is the time duration, \( \epsilon_R \) and \( \epsilon_T \) are the axial strains obtained from the reflected and transmitted pulses, respectively.

The true stress, true strain and true strain-rate in the specimen \cite{102} are given by

\[
\sigma_s = \sigma_s(t)[1 - e_s(t)] \\
\epsilon_s(t) = -\ln[1 - e_s(t)] \\
\dot{\epsilon}_s = \frac{\dot{\epsilon}_s(t)}{1 - e_s(t)}
\]  

(7.4) \hspace{1cm} (7.5) \hspace{1cm} (7.6)

### 7.1.2 Strain gauge output

The raw output obtained from strain gauges mounted on the incident and transmission bars for single crystal copper deformed at \( \sim 10^4 \) s strain rate is shown in Figure 7.2(a). The strain and stress produced in the specimen due to the impact of striker bar on the incident bar are obtained by using the following relations \cite{103}

\[
\epsilon = \frac{2\Delta V}{V_0 k G} \\
\sigma = \frac{2\Delta V E}{V_0 k G}
\]  

(7.7) \hspace{1cm} (7.8)

where \( \Delta V \) is the signal from the strain gauges mounted on the bars, \( E \) is the elastic modulus of the bar, \( V_0 \) is the excitation voltage, \( k \) is the gage factor and \( G \) is the gain.

The incident, reflected and transmitted stress waves are shown in Figure 7.2(b).
Figure 7.2: (a) Strain gauge raw output obtained from incident and transmission bars for high strain rate test on single crystal copper at room temperature for an impact velocity of 9.4 m/s in SHPB (b) Strain gauge raw output converted to stress for the impact velocity of 9.4 m/s.
7.1.3 Maximum stress generated in the incident bar and pulse duration

The maximum stress generated due to the impact of the striker bar on the incident bar is given by [104]

\[ \sigma_{\text{max}} = \frac{\rho c_0 v}{2} \]  \hspace{1cm} (7.9)

where \( v \) is the velocity of the striker bar, \( \rho \) (7746 kg/m\(^3\)) is the density of the pressure bars and \( c_0 \) (4793 m/s) is the elastic wave velocity in the pressure bars.

For an impact velocity of 9.4 m/s, the maximum stress generated is given by

\[ \sigma_{\text{max}} = \frac{7746 \times 4793 \times 9.4}{2} = 174\text{MPa} \]  \hspace{1cm} (7.10)

This is in agreement with the maximum stress obtained from the experiment on single crystal copper, as shown in Figure 7.2 (b).

The duration of the pulse generated is given by

\[ \Delta t = \frac{2L}{c_0} = \frac{2 \times 0.5}{4793} = 208\mu \text{s} \]  \hspace{1cm} (7.11)

where \( L \) is the length of the striker bar. The pulse duration calculated is also in agreement with that obtained from the experiment, as shown in Figure 7.2 (b).

7.2 Experimental Procedure

7.2.1 Preparation of single crystal specimens for SHPB

A single crystal copper of dimension 25.0 mm (diameter) \( \times \) 20.0 mm (height) was grown by Bridgman method\(^1\) (Figure 7.3). The neutron diffraction method has been used to determine the crystalline perfection and orientation of the copper sample. The instruments used were a Triple Axis Neutron Spectrometer (TAS) [105], and a Filter Detector Neutron Spectrometer (FDS) at Dhruva reactor, BARC. In these spectrometers, the (111) reflection of large copper single crystals are used to obtain a monochromatic neutron beam. The collimator in the monochromatic beam allows a beam cross section of 5.0 cm \( \times \) 5.0 cm onto the sample and the horizontal divergence would be 1\(^\circ\) [106].

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\(^1\) Single crystal copper is provided by Prof. Thamizhavel from Tata Institute of Fundamental Research (TIFR), Mumbai, India. This contribution is gratefully acknowledged.
The methodology employed is the measurement of a neutron diffraction rocking curve. This is the measurement of the intensity of an "hkl" reflection as the crystal is turned around its vertical axis, in order to characterize the quality of the crystal regarding its mosaicity $\Delta\theta$ – the planes that theoretically should be parallel to each other differ in reality by an angle $\Delta\theta$. In general, this rocking curve shows overlapping peaks if crystalline domains (closely aligned in the direction of measurement) are present in the crystal.

During the measurement, the neutron detector remains in a fixed position at the scattering angle $2\theta_{hkl}$ relative to the incident beam. The wavelength of the neutrons used was 2.3 Å. The crystal to be investigated was attached firmly to the head of a two-axis goniometer, with the cylinder axis vertical. The goniometer was then placed on the sample table of the spectrometer. Careful orientation of the crystal in the neutron beam was carried out in order to obtain the maximum intensity of the (111) and (200) reflections. The rocking curve was obtained by rotating the crystal in steps of 0.1° with a count time of 10 s for each step. The determined orientation of the copper crystal has helped in marking the <100> direction as well as confirming the <011>/<011> to be along the axis of the cylinder. The direction marked crystal copper is shown in Figure 7.4.

The rocking curve of the (200) reflection measured on the FDS is shown in Figure 7.5. In Figure 7.5, it is seen that only two good peaks are observed during the whole rotation of the sample. These peaks indicate that the single crystal copper is not a polycrystalline copper. In the inset of Figure 7.5, an expanded scale of the counts (intensity) axis is also shown. In the inset, it is seen that there are small
peaks in between the two good (big) peaks. The presence of small peaks between the two big peaks signifies the presence of crystallites which are not aligned with the main ones. The rocking curve of (111) reflection (Figure 7.6) also shows the presence of small peaks in-between the big peaks. The rocking curve of the (200) reflection with an expanded scale of sample angle axis is shown in Figure 7.7. A Gaussian fit of the data (Figure 7.7) gives the width to be around 0.9°, which is a measure of the mosaicity of the crystal.

7.2.2 Energy Dispersive X-ray (EDX) Analysis

This technique is used to identify impurities in the specimen. In this technique, an electron beam is used to bombard the specimen. These electrons collide with atoms of different elements present in the specimen. Due to collisions with bombarded electrons, the inner shell electrons in the sample are ejected, leading to vacant positions in the inner shells. These vacant positions are occupied by the high energy electrons from the outer shells of the atoms. The transfer of outer shell electrons to inner shells leads to the release of energy by emitting X-rays. The amount of energy released depends on the energy difference between the energy levels (energy level from where the electron is ejected and that from which the electron is transferred to
occupy the vacant position). The atoms of each element emit X-rays with a unique amount of energy. The measurement of amount of energy present in X-rays is used to identify the atoms present in the specimen.

The EDX spectrum for single crystal copper is shown in Figure 7.8. It is seen in Figure 7.8 that each of the peaks is unique to an atom and hence corresponds to a single element. As expected, the copper peak is the highest, which is a signature of high concentration of the element present in the specimen. Only a few impurities (C, O, Cl and Si) are present in the single crystal copper.

### 7.3 Johnson-Cook Material Model

The Johnson-Cook (JC) model [27] is a phenomenological model used to reproduce the response of the materials under impact and penetration conditions. The model connects the quasi-static and dynamic mechanical properties of the materials. The material responses which are described by this model are strain hardening, strain rate effect and thermal softening. In this model, the equivalent von Mises stress is
Figure 7.6: Rocking curve of (111) reflection for single crystal copper (Figure 7.3).

given by

\[
\sigma_e = [A + B(\varepsilon_p^e)^n][1 + C\ln \dot{\varepsilon}][1 - T^* m]
\]

(7.12)

where A is the quasi-static yield stress, B is the modulus of strain hardening, \( n \) is
the strain hardening exponent, C is the strain rate hardening constant and \( m \) is the
thermal softening constant, all of which are material constants. \( \varepsilon_p^e \) is the equivalent
plastic strain, \( \dot{\varepsilon}^* = \frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \) is the plastic strain rate, \( \dot{\varepsilon}_0 \) is the user-defined reference strain
rate used to determine A, B, and \( n \).

\[
T^* = \frac{T - T_R}{T_M - T_R}
\]

is the dimensionless temperature called the homologous temperature, \( T_M \) is the
melting temperature and \( T_R \) is the reference temperature (room temperature) used
to determine A, B and \( n \).

There are three terms in parentheses on the right hand side of Eqn. 7.12:

- The first term \([ A + B (\varepsilon_p^e)^n ]\) represents the material properties under quasi-
  static loading.

- The second term \([ 1 + C \ln \dot{\varepsilon}^* \]) describes the effect of strain-rate hardening.
Figure 7.7: Rocking curve of (111) reflection for single crystal copper (Figure 7.3)

- The third term \([1 - T^m]\) describes the thermal softening effect due to imposed temperature.

If thermal softening effects are ignored, i.e. \(T^* = 0\) for \(T = T_R\), then Eqn. 7.12 becomes

\[
\sigma_e = [A + B(\dot{\varepsilon}_e^p)^n][1 + C \ln \dot{\varepsilon}^*] \quad (7.13)
\]

If strain-rate effect and thermal softening effects are ignored, i.e. \(\dot{\varepsilon}^* = 1.0\) and \(T^* = 0\), then Eqn. 7.12 becomes

\[
\sigma_e = [A + B(\dot{\varepsilon}_e^p)^n] \quad (7.14)
\]

This describes the relationship between stress and strain under quasi-static loading.

### 7.4 Results and Discussion

To determine the strength properties, quasi-static experiments using Universal Testing Machine (UTM) and dynamic experiments using SHPB have been performed on single crystal copper loaded along <100> and <110> directions. The details of
Figure 7.8: EDX spectrum for single crystal copper.

the quasi-static and dynamic compression experiments on single crystal copper are shown in Table 7.1 and Table 7.2, respectively.

<table>
<thead>
<tr>
<th>Test No</th>
<th>Specimen size L×D (mm)</th>
<th>Orientation</th>
<th>Strain rate (/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.94×4.04</td>
<td>100</td>
<td>0.0033</td>
</tr>
<tr>
<td>2</td>
<td>3.96×4.06</td>
<td>110</td>
<td>0.0033</td>
</tr>
</tbody>
</table>

Table 7.1: Experimental details for single crystal copper deformed under quasi-static loading at 300 K.

A comparison of true stress as a function of true strain for <100> and <110> loading directions under quasi-static loading is shown in Figure 7.9.
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<table>
<thead>
<tr>
<th>Test No.</th>
<th>Specimen size L×D (mm)</th>
<th>Orientation</th>
<th>Temperature (K)</th>
<th>Gas gun pressure (bar)</th>
<th>Striker bar velocity (m/s)</th>
<th>Average strain rate (/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.88×4.04</td>
<td>100</td>
<td>300</td>
<td>1.5</td>
<td>9.38</td>
<td>2300</td>
</tr>
<tr>
<td>2</td>
<td>3.94×4.08</td>
<td>100</td>
<td>300</td>
<td>2.0</td>
<td>11.72</td>
<td>3000</td>
</tr>
<tr>
<td>3</td>
<td>3.94×4.06</td>
<td>100</td>
<td>300</td>
<td>2.5</td>
<td>13.33</td>
<td>3500</td>
</tr>
<tr>
<td>4</td>
<td>3.96×4.0</td>
<td>100</td>
<td>373</td>
<td>2.0</td>
<td>11.72</td>
<td>3000</td>
</tr>
<tr>
<td>5</td>
<td>3.96×4.0</td>
<td>100</td>
<td>473</td>
<td>2.0</td>
<td>11.72</td>
<td>3000</td>
</tr>
<tr>
<td>6</td>
<td>4.00×4.10</td>
<td>110</td>
<td>300</td>
<td>1.5</td>
<td>9.38</td>
<td>2200</td>
</tr>
<tr>
<td>7</td>
<td>3.94×4.10</td>
<td>110</td>
<td>300</td>
<td>2.5</td>
<td>13.33</td>
<td>3500</td>
</tr>
<tr>
<td>8</td>
<td>3.96×4.10</td>
<td>110</td>
<td>300</td>
<td>3.0</td>
<td>14.71</td>
<td>4200</td>
</tr>
<tr>
<td>9</td>
<td>4.0×4.02</td>
<td>110</td>
<td>373</td>
<td>2.0</td>
<td>11.72</td>
<td>3000</td>
</tr>
<tr>
<td>10</td>
<td>3.94×4.0</td>
<td>110</td>
<td>473</td>
<td>2.0</td>
<td>11.72</td>
<td>3000</td>
</tr>
</tbody>
</table>

Table 7.2: Experimental details for single crystal copper deformed under dynamic loading using SHPB.

Figure 7.9: Comparison of true stress-true strain curves for single crystal copper deformed along <100> and <110> directions under quasi-static loading.
It is seen in Figure 7.9 that single crystal copper, deformed along the \(<100>\) direction, shows more hardening than that deformed along \(<100>\) direction.

True stress as a function of true strain at different strain rates is shown in Figure 7.10. Note that the strain rate under dynamic loading is not constant during the deformation.

![Graphs showing true stress-strain relationship for different strain rates and crystal orientations](image)

**Figure 7.10:** Deformation of single crystal copper at 300 K using UTM and SHPB. (a) True stress as a function of true strain for single crystal copper deformed along \(<100>\) direction (b) True strain rate-true strain curve for loading along \(<100>\) direction (c) True stress-true strain curve for loading along \(<110>\) direction (d) True strain rate-true strain curve for loading along \(<110>\) direction.

The quasi-static data for single crystal copper is used to get three parameters (A, B and n) for the JC model. The strain rate coefficient (C) is obtained by using stress-strain data at different strain rates, while the thermal softening coefficient (m) is obtained by using stress-strain data at different temperatures for a constant strain rate. JC model parameters for single crystal copper deformed along \(<100>\) and \(<110>\) directions are shown in Table 7.3. For experiments performed at room
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<table>
<thead>
<tr>
<th>JC model parameters</th>
<th>Orientation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>&lt;100&gt;</td>
</tr>
<tr>
<td>A (MPa)</td>
<td>35.0</td>
</tr>
<tr>
<td>B (MPa)</td>
<td>355.3</td>
</tr>
<tr>
<td>n</td>
<td>0.46</td>
</tr>
<tr>
<td>C</td>
<td>0.022</td>
</tr>
<tr>
<td>m</td>
<td>0.85</td>
</tr>
</tbody>
</table>

Table 7.3: JC model parameters for single crystal copper deformed at $10^3/s$ strain rate along <100> and <110> directions.

Temperature (i.e., $T = T_R$), Eqn. 7.13 becomes

$$
\sigma_e = \begin{cases} 
[35.0 + 355.3(\dot{\varepsilon}^*)^{0.46}] [1 + 0.022 \ln \dot{\varepsilon}^*] & for \ <100> \\
[55.0 + 537.8(\dot{\varepsilon}^*)^{0.62}] [1 + 0.0009 \ln \dot{\varepsilon}^*] & for \ <110>
\end{cases}
$$

(7.15)

For single crystal copper deformed along <100> and <110> directions, a comparison of true stress-true strain curves obtained from experiments and that using Eqn. 7.15 is shown in Figure 7.11.
Figure 7.11: Comparison of true stress-true strain curves obtained from experiments and that using Eqn. 7.15 for single crystal copper deformed at $10^3/\text{s}$ strain rate along (a) $<100>$ direction (b) $<110>$ direction.

As mentioned above, by performing experiments at different temperatures at constant average strain rate, the thermal softening coefficient is determined. Therefore, Eqn. 7.13 becomes

$$\sigma_e = \begin{cases} 
35.0 + 355.3(\epsilon^*_p)^{0.46}[1 + 0.022 \ln \epsilon^*_p][1 - T^{*0.85} ] & \text{for } <100> \\
55.0 + 537.8(\epsilon^*_p)^{0.62}[1 + 0.0009 \ln \epsilon^*_p][1 - T^{*0.9}] & \text{for } <110> 
\end{cases} \quad (7.16)$$
Comparison of true stress-true strain curves obtained from experiments and that using Eqn. 7.16 for single crystal copper deformed along $<100>$ and $<110>$ directions at different temperatures and different strain rates is shown in Figure 7.12.

![Figure 7.12](image)

**Figure 7.12:** Comparison of true stress-true strain curves obtained from experiments and that using Eqn. 7.16 for single crystal copper deformed at $10^3$/s strain rate along (a) $<100>$ direction (b) $<110>$ direction.

It can be seen from Figure 7.12 that there is good agreement between the stress-strain curves obtained by experiments and that obtained using Eqn. 7.16.
7.5 Estimation of dislocation density

To estimate the dislocation density in single crystal copper, neutron diffraction analysis has been carried out before and after the deformation of single crystal copper at $10^3$/s strain rate. The analysis has been done for single crystal copper deformed along $<100>$ direction. The neutron diffraction analysis method is described in Section 7.2.1.

The true stress-true strain curves and true strain rate-true strain curves for two specimens (specimen 12 and specimen 13), deformed at two impact velocities of the striker bar, are shown in Figure 7.13.

![Figure 7.13](image)

**Figure 7.13:** (a) True stress-true strain curves for specimen 12 and specimen 13 (b) True strain-rate as a function of true strain for specimen 12 and specimen 13.
The rocking curves of (200) and (220) reflections for specimen 12 and specimen 13, before and after the deformation, are shown in Figure 7.14.

The full width at half maximum (FWHM) for specimen 12 and specimen 13, before and after the deformation, is calculated using the rocking curves as shown in Figure 7.15 and Figure 7.16, respectively.

**Figure 7.14:** Rocking curve of (a) (200) reflections for specimen 12 (b) (220) reflections for specimen 12 (c) (200) reflections for specimen 13 (d) (220) reflections for specimen 13.

Assuming a random distribution of the dislocations on all possible slip systems, the average dislocation density \( D \) [107] is given by

\[
D = \frac{\beta^2}{9b^2} \quad (7.17)
\]

where \( \beta \) is the FWHM of the rocking curves measured by neutron diffraction, and \( b \) is the Burger vector (here \( b = \frac{a}{2} \langle 110 \rangle = 0.255 \text{ nm}, a = 0.361 \text{ nm} \)). Using Eqn. 7.17, the dislocation density for single crystal copper deformed along \( \langle 100 \rangle \) and \( \langle 110 \rangle \) directions is shown in Table 7.4.
Figure 7.15: FWHM for specimen 12 (a) before deformation for (200) reflections (b) after deformation for (200) reflections (c) before deformation for (220) reflections and (d) after deformation for (220) reflections. Specimen 12 is deformed at $10^3$/s (Figure 7.13) along <100> crystal direction.

### 7.6 Molecular dynamics simulation

To understand the shape changes observed in experiments on single crystal copper and to reproduce the number of active slip directions during deformation of single crystal copper loaded along <100> and <110> directions, MD simulations have been performed at high strain rate under uniaxial stress loading.

The simulation domain contains $100 \times 100 \times 100$ unit cells along x-, y- and z-directions. Periodic boundary conditions are used along each direction. Equations of motion are integrated with a time step of 0.5 femto-second using velocity Verlet algorithm. After relaxing the system at 300 K temperature and 0 bar pressure for 100 pico-second, uniaxial compression at $5 \times 10^9$/s strain rate has been applied along the x-direction. The pressure along y- and z-directions has been controlled at 0
Figure 7.16: FWIM for specimen 13 (a) before deformation for (200) reflections (b) after deformation for (200) reflections (c) before deformation for (220) reflections and (d) after deformation for (220) reflections. Specimen 13 is deformed at $10^3$/s (Figure 7.13) along $<100>$ crystal direction.

pressure using an NPT ensemble, thereby letting the solid change shape and size along these directions.

### 7.6.1 Number of slip systems activated

Single crystal copper uniaxially compressed along $<100>$ and $<110>$ directions at $5 \times 10^9$/s strain rate first deforms elastically and then plastically once the threshold for dislocation nucleation is crossed. The deformation along the $<100>$ direction leads to the activation of 8 slip systems and that along the $<110>$ direction activates 4 slip systems [108] out of 12 active slip systems in FCC metals. In order to study the slip systems activated during dynamic deformation, Burger vectors have been calculated using the DXA code [109]. These Burger vectors are then used to get
Table 7.4: FWHM and average dislocation density for specimen 12 and specimen 13 before and after the deformation of single crystal copper obtained from rocking curves (Figure 7.15 and Figure 7.16).

the slip directions. The number of slip directions activated in single crystal copper deformed along <100> and <110> directions are shown in Figure 7.17.

It is seen in Figure 7.17 (a) that there are 8 sets of h, k and l values which indicate the activation of 8 slip directions. In Figure 7.17 (b), there are 4 sets of h, k and l values which indicate the activation of 4 slip directions in single crystal copper deformed along <110> direction. This reproduces the number of active slip directions observed by [108].
Figure 7.17: Number of slip directions activated during deformation of perfect single crystal copper at 5×10^9/s strain rate with 300K along (a) <100> direction (b) <110> direction.

7.6.2 Shape changes in the deformation of single crystal copper

The Poisson ratio as a function of strain for single crystal copper deformed at 5×10^9/s strain rate along <100> and <110> directions is shown in Figure 7.18.
Figure 7.18: Poisson ratio as a function of strain in the direction of compression for single crystal copper deformed at $5 \times 10^3$ strain rate along (a) $<100>$ direction (b) $<110>$ direction.

The arrow in Figure 7.18 indicates the onset of plastic deformation due to homogeneous nucleation of dislocations. It is seen in Figure 7.18 (a) that for $<100>$ loading direction, the Poisson ratio is negative for both y- and z-directions. This indicates the expansion of the crystal along y- and z-directions due to compression along x-direction. This supports the shape changes observed in experiments on cylindrical single crystal copper specimens loaded along $<100>$ direction. The
image of single crystal copper specimen deformed along $<100>$ direction at $10^3$/s strain rate using SHPB is shown in Figure 7.19(a).

For loading along the $<110>$ direction, the Poisson ratio is positive along the y-direction and negative along the z-direction, as shown in Figure 7.18(b). This indicates that during elastic deformation, the crystal contracts along the y-direction and expands along the z-direction due to compression in x-direction. Note that deformation of single crystal copper is large along the z-direction compared to y-direction. Note also that during plastic deformation, single crystal copper expands along both y- and z-directions, but with larger deformation along the z-direction. The image of the specimen deformed along $<110>$ direction at $10^3$/s strain-rate using SHPB is shown in Figure 7.19(b).

Thus, the shape changes observed in SHPB experiments on single crystal copper are validated by MD simulations.

![Image](image1.png)

(a) \hspace{1cm} (b)

**Figure 7.19:** Single crystal copper deformed at $10^3$/s strain rate using SHPB along (a) $<100>$ direction (b) $<110>$ direction.

To understand the shape changes of the above samples, Schmid factor calculations have been performed on the (111) slip plane to determine the activation of slip directions. It is known that shear stresses are produced when load is applied on the material [110]. The shear stress produced leads to slip in the material if it reaches a threshold value called critical resolved shear stress (CRSS). The critical resolved shear stress ($\tau$) is given by

$$\tau_R = \sigma \cos \phi \cos \lambda$$  \hspace{1cm} (7.18)

where $\sigma$ is the axial stress, $\phi$ is the angle between normal to slip plane and the ten-
sion/compression axis, \( \lambda \) is the angle between slip direction and tension/compression direction. Here \( \cos \phi \cos \lambda \) is called the Schmid factor (m). The value of Schmid factor determines activation of the slip systems. The slip systems which have highest Schmid factor will activate first.

**Shape changes when deformed along \(<100>\) direction**

For \( <111> \) slip plane and \(<100>\) compression axis, the angle between the two is given by

\[
\cos \phi = \frac{(1)(1) + (1)(0) + (1)(0)}{\sqrt{1^2 + 1^2 + 1^2} \sqrt{1^2 + 0^2 + 0^2}} = \frac{1}{\sqrt{3}}
\]  
(7.19)

The slip plane \( <111> \) contains three slip directions: \(<\bar{1}10>\), \(<\bar{1}01>\) and \(<0\bar{1}1>\). Therefore, the angle between slip directions and the compression axis \(<100>\) is given by

\[
\cos \lambda = \frac{(\bar{1})(1) + (1)(0) + (0)(0)}{\sqrt{(\bar{1})^2 + 1^2 + 0^2 \sqrt{1^2 + 0^2 + 0^2}}} = \frac{1}{\sqrt{2}} \quad \text{for } <\bar{1}10> \tag{7.20}
\]

\[
\cos \lambda = \frac{(\bar{1})(1) + (0)(0) + (1)(0)}{\sqrt{(\bar{1})^2 + 0^2 + 1^2 \sqrt{1^2 + 0^2 + 0^2}}} = -\frac{1}{\sqrt{2}} \quad \text{for } <\bar{1}01> \tag{7.21}
\]

\[
\cos \lambda = \frac{(0)(1) + (\bar{1})(0) + (1)(0)}{\sqrt{0^2 + (\bar{1})^2 + 1^2 \sqrt{1^2 + 0^2 + 0^2}}} = 0 \quad \text{for } <0\bar{1}1> \tag{7.22}
\]

Therefore, the Schmid factor (m) for \(<\bar{1}10>\) slip direction is given by

\[
m_{<\bar{1}10>} = \cos \phi \cos \lambda = \left(\frac{1}{\sqrt{3}}\right)(\frac{1}{\sqrt{2}}) = \frac{1}{\sqrt{6}} = -0.408
\]  
(7.23)

Similarly, for \(<\bar{1}01>\) and \(<0\bar{1}1>\) slip directions, the Schmid factor is given by

\[
m_{<\bar{1}01>} = \cos \phi \cos \lambda = \left(\frac{1}{\sqrt{3}}\right)(-\frac{1}{\sqrt{2}}) = -\frac{1}{\sqrt{6}} = -0.408
\]  
(7.24)

\[
m_{<0\bar{1}1>} = \cos \phi \cos \lambda = \left(\frac{1}{\sqrt{3}}\right)(0) = 0
\]  
(7.25)

It is seen from Eqn. 7.23 and Eqn. 7.24 that the Schmid factor for \(<\bar{1}10>\) and \(<\bar{1}01>\) is equal and non-zero, which means that both these slip directions will activate simultaneously. For \(<0\bar{1}1>\) slip direction, the Schmid factor is zero which means that no slip will occur along this direction since there is no shear stress along this direction (Eqn. 7.18). This is the reason why single crystal copper expands along y-
and z-directions when deformed along <100> direction (x-direction). The graphical representation of activation of slip directions on 4 active slip planes for single crystal copper deformed along <100> direction is shown in Figure 7.20 and the details of the slip systems are tabulated in Table 7.5.

![Graphical representation of activation of slip directions on 4 active slip planes for single crystal copper deformed along <100> direction.](image)

**Figure 7.20:** Graphical representation of activation of slip directions on 4 active slip planes for single crystal copper deformed along <100> direction.

**Shape changes when deformed along <110> direction**

The angle between (111) slip plane and <110> slip direction is given by

\[
\cos \phi = \frac{(1)(1) + (1)(1) + (1)(0)}{\sqrt{1^2 + 1^2 + 1^2} \sqrt{1^2 + 0^2 + 0^2}} = \frac{2}{\sqrt{6}}
\]  

(7.26)
<table>
<thead>
<tr>
<th>Slip plane normal (n)</th>
<th>cos φ (n.c)</th>
<th>Slip direction (s)</th>
<th>cos λ (s.c)</th>
<th>Schmid factor (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(111)</td>
<td>0.577</td>
<td>&lt;\overline{1}10&gt;</td>
<td>-0.707</td>
<td>-0.408</td>
</tr>
<tr>
<td></td>
<td></td>
<td>&lt;\overline{1}01&gt;</td>
<td>-0.707</td>
<td>-0.408</td>
</tr>
<tr>
<td>(1\overline{1}1)</td>
<td>0.577</td>
<td>&lt;\overline{1}01&gt;</td>
<td>-0.707</td>
<td>-0.408</td>
</tr>
<tr>
<td></td>
<td></td>
<td>&lt;\overline{1}10&gt;</td>
<td>-0.707</td>
<td>-0.408</td>
</tr>
<tr>
<td>(1\overline{1}1)</td>
<td>0.577</td>
<td>&lt;\overline{1}01&gt;</td>
<td>-0.707</td>
<td>-0.408</td>
</tr>
<tr>
<td></td>
<td></td>
<td>&lt;\overline{1}10&gt;</td>
<td>-0.707</td>
<td>-0.408</td>
</tr>
</tbody>
</table>

Table 7.5: All 8 slip systems which activate during the deformation of single crystal copper when deformed along <100> direction. Here c indicates the direction of compression (<100>).

The angle between slip directions (<\overline{1}10>, <\overline{1}01> and <0\overline{1}1>) and compression axis (<110>) is given by

$$\cos \lambda = \frac{\langle \overline{1} \rangle(1) + (1)(1) + (0)(0)}{\sqrt{(1)^2 + 1^2 + 0^2 \sqrt{1^2 + 1^2 + 0^2}}} = \frac{0}{\sqrt{6}} = 0 \quad for \ <\overline{1}10> \quad (7.27)$$

$$\cos \lambda = \frac{\langle \overline{1} \rangle(1) + (0)(1) + (1)(0)}{\sqrt{(1)^2 + 0^2 \sqrt{1^2 + 1^2 + 0^2}}} = \frac{-1}{\sqrt{4}} = -\frac{1}{2} \quad for \ <\overline{1}01> \quad (7.28)$$

$$\cos \lambda = \frac{(0)(1) - \langle \overline{1} \rangle(1) + (1)(0)}{\sqrt{0^2 + (1)^2 + 1^2 \sqrt{1^2 + 1^2 + 0^2}}} = \frac{-1}{\sqrt{4}} = -\frac{1}{2} \quad for \ <0\overline{1}1> \quad (7.29)$$

Therefore, the Schmid factor for <\overline{1}10>, <\overline{1}01> and <0\overline{1}1> slip directions is given by

$$m_{<\overline{1}10>} = \cos \phi \cos \lambda = \left(\frac{2}{\sqrt{6}}\right)(0) = 0 \quad (7.30)$$

$$m_{<\overline{1}01>} = \cos \phi \cos \lambda = \left(\frac{2}{\sqrt{6}}\right)(-\frac{1}{2}) = -\frac{1}{\sqrt{6}} = -0.408 \quad (7.31)$$

$$m_{<0\overline{1}1>} = \cos \phi \cos \lambda = \left(\frac{2}{\sqrt{6}}\right)(-\frac{1}{2}) = -\frac{1}{\sqrt{6}} = -0.408 \quad (7.32)$$
It is seen in Eqn. 7.30 that the Schmid factor is zero for \(<\overline{1}10>\) slip direction, while it is non-zero for \(<\overline{1}0\overline{1}>\) and \(<0\overline{1}1>\) slip directions. Therefore, slip will occur along \(<\overline{1}0\overline{1}>\) and \(<0\overline{1}1>\) directions leading to expansion along \(z\)-direction. This is the reason why more deformation takes place along \(z\)-direction. The graphical representation of activation of slip directions on 2 active slip planes for single crystal copper deformed along \(<110>\) direction is shown in Figure 7.21 and details of the slip systems are tabulated in Table 7.6.

**Figure 7.21:** Graphical representation of activation of slip directions on 2 active slip planes for single crystal copper deformed along \(<110>\) direction.
<table>
<thead>
<tr>
<th>Slip plane normal ( (n) )</th>
<th>Slip direction ( (s) )</th>
<th>( \cos \phi ) ( (n,c) )</th>
<th>( \cos \lambda ) ( (s,c) )</th>
<th>Schmid factor ((m))</th>
</tr>
</thead>
<tbody>
<tr>
<td>((111))</td>
<td>(&lt;\overline{1}0\overline{1}&gt;)</td>
<td>0.816</td>
<td>-0.50</td>
<td>-0.408</td>
</tr>
<tr>
<td>&amp; (&lt;0\overline{1}1&gt;)</td>
<td>&amp; -0.50</td>
<td>&amp; -0.408</td>
<td></td>
<td></td>
</tr>
<tr>
<td>((1\overline{1}1))</td>
<td>(&lt;\overline{1}0\overline{1}&gt;)</td>
<td>0.816</td>
<td>-0.50</td>
<td>-0.408</td>
</tr>
<tr>
<td>&amp; (&lt;0\overline{1}1&gt;)</td>
<td>&amp; -0.50</td>
<td>&amp; -0.408</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 7.6: All 4 slip systems which activate during the deformation of single crystal copper when deformed along \(<110>\) direction. Here \(c\) indicates the direction of compression \((<110>)\).

## 7.7 Conclusions

The conclusions are as follows:

- The strength parameters for Johnson-Cook model have been obtained for single crystal copper deformed at \(10^3/s\) strain rate along \(<100>\) and \(<110>\) directions. The value of yield strength and strain hardening parameter for single crystal copper deformed along the \(<110>\) direction is high compared to that deformed along the \(<100>\) direction.

- Neutron diffraction studies before and after the impact show the broadening of the diffraction peaks which is the signature of increased density of defects. The change in the diffraction peaks have been correlated with dislocations in the sample.

- Using MD simulations, the number of slip directions activated during the deformation of single crystal copper has been reproduced by computing the Burger vector for homogeneous nucleation of dislocations. Furthermore, shape changes observed in the experiments on single crystal copper have been validated by computing the Poisson ratio. The shape changes are understood in terms of the activation of preferred slip systems by performing the Schmid factor calculations.