## strain fit

#### November 4, 2024

# 1 Calculate reference stress for each temperature at each strain rate

For each condition, calculate take the stress where strain is smaller than 0.08 and divide it by the reference stress at  $298.15 \mathrm{K}$ 

```
[]: import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from scipy.optimize import curve_fit
from sklearn.metrics import r2_score
from itertools import product # Import product for grid search
```

```
[]: def organise_data(strain_rates, temps):
         ref_temp = '298.15'
         for temp in temps:
             # Initialize DataFrame with strain column for the current temperature
             df = None # Initialize df to None to handle it dynamically for each
      \hookrightarrow temperature
             for strain_rate in strain_rates:
                 # Load stress data for the current temperature and strain rate
                 data_RD = pd.read_csv(f'../extended_curve/
      →Tmp{temp}K_StrRt{strain_rate}_RD.csv')
                 if df is None:
                     # Initialize DataFrame with strain column if not already done
                     df = pd.DataFrame({'strain': data_RD['Strain']})
                 # Add stress data for the current strain rate as a new column
                 df[f'StrRt{strain_rate}'] = data_RD['Stress']
             # Filter the DataFrame for strain values below 0.08
             df = df[df['strain'] < 0.08]</pre>
             # Save the DataFrame to a CSV file for the current temperature
             output_file_path = f"Tmp{temp}_RD.csv"
```

```
df.to_csv(output_file_path, index=False)
```

```
[]: #First set, not necessary
strain_rates = [0.0001]
temps = ['77.15', '233.15']
organise_data(strain_rates, temps)

#Second set
strain_rates = [0.0001, 0.001, 0.01, 0.1]
temps = ['373.15', '473.15', '573.15', '673.15']
organise_data(strain_rates, temps)

#Third set
strain_rates = [0.0001, 0.001, 0.01, 0.1,1]
temps = ['298.15']
organise_data(strain_rates, temps)
```

# 2 Find parameters for strain rate function

```
[]: def fit_strain_rate_dependency(temperature_file, strain_rates,__
      ⇔strain_rate_columns):
         Fits strain rate dependency for each row in a dataset and exports results.
         Parameters:
         - temperature file (str): Path to the CSV file containing the data for all
      \hookrightarrow specific temperature.
         - strain_rates (list of float): List of strain rate values corresponding to \Box
      \hookrightarrow columns in the dataset.
          - strain_rate_columns (list of str): List of column names in the data⊔
      ⇔corresponding to strain rates.
         Output:
         - CSV file with columns: PEEQ, C1, C2, R_squared for each row in the \sqcup
      \hookrightarrow dataset.
         # Load the temperature-specific file
         data = pd.read_csv(f"{temperature_file}.csv")
         # Default rows to plot
         plot_indices = [3, 4, 5, 6, 11]
         # Define a scaling factor for better readability in the plot legend
         scale_factor = 1e8
         # Define the strain-rate dependency function
```

```
def strain rate dependent stress(strain rate, C1, C2, stress_values):
      return np.array([s * (C1 * np.log(sr) + C2) for s, sr in_
⇒zip(stress_values, strain_rate)])
  # List to store the results
  results = []
  # Loop through all rows in the dataset for strain-rate dependency fitting
  for i in range(len(data)):
       # Extract stress data for the specified strain rates at row `i`
      stress_values = data.iloc[i][strain_rate_columns].values # Select_
⇔specified strain rate columns
      plastic_strain = data['strain'].iloc[i] # Get the plastic strain at_
→ this row (PEEQ)
       # Fit strain-rate dependency with evolving stress values
      initial_guess_sr = [0.1, 1] # Adjusted initial guesses
      bounds sr = ([0, 0], [np.inf, np.inf]) # Tighter bounds to avoid
⇔non-physical values
       # Perform the curve fitting for strain-rate dependency using evolving
⇔stress values
      try:
          params_sr, _ = curve_fit(lambda sr, C1, C2:__
strain_rate_dependent_stress(sr, C1, C2, stress_values),
                                    strain rates, stress values,
⇒p0=initial_guess_sr, bounds=bounds_sr)
       except RuntimeError:
          print(f"Could not fit strain-rate dependency for row {i}")
          continue
       # Calculate residuals for error estimation
      stress_fit = strain_rate_dependent_stress(strain_rates, *params_sr,_
⇔stress values)
      residuals = stress_values - stress_fit
      ss_res = np.sum(residuals**2)
      ss_tot = np.sum((stress_values - np.mean(stress_values))**2)
      r_squared = 1 - (ss_res / ss_tot)
       # Store results for exporting
      results.append({
           "PEEQ": plastic_strain,
           "C1": params_sr[0],
           "C2": params_sr[1],
           "R_squared": r_squared
      })
```

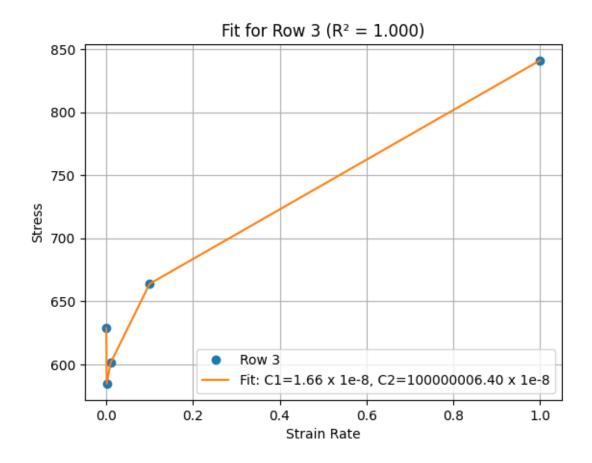
```
# Plot only for specified rows with scaled C1 and C2 in legend
if i in plot_indices:
    plt.plot(strain_rates, stress_values, 'o', label='Data')
    plt.plot(strain_rates, stress_fit, '-', label='Fit') # Use only_

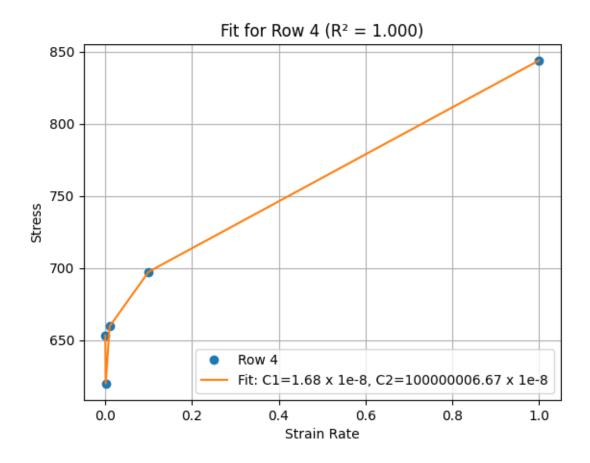
original strain rates for fit plot
    plt.xlabel('Strain Rate')
    plt.ylabel('Stress')
    plt.title(f"Fit for Row {i} (R² = {r_squared:.3f})")
    plt.legend([f'Row {i}', f'Fit: C1={params_sr[0] * scale_factor:.2f}_

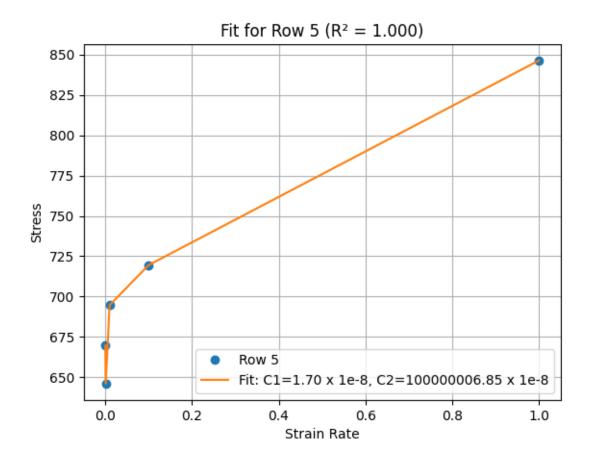
x 1e-8, C2={params_sr[1] * scale_factor:.2f} x 1e-8'], loc="lower right")
    plt.grid()
    plt.show()

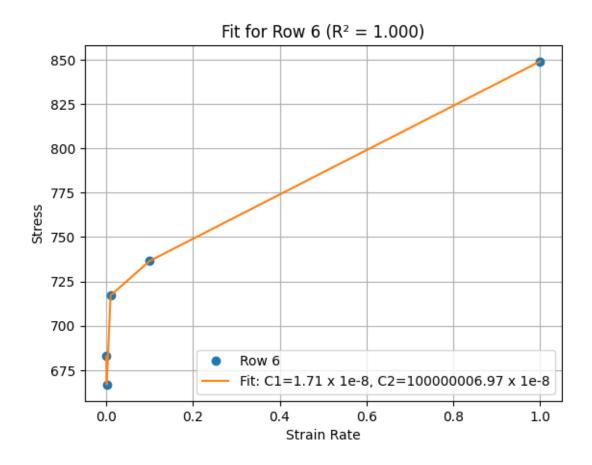
# Export results to CSV
results_df = pd.DataFrame(results)
results_df.to_csv(f"Parameters_{temperature_file}.csv", index=False)
```

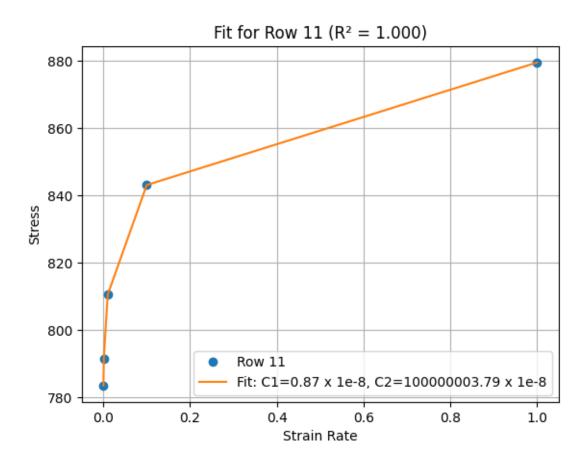
#### 2.1 RT



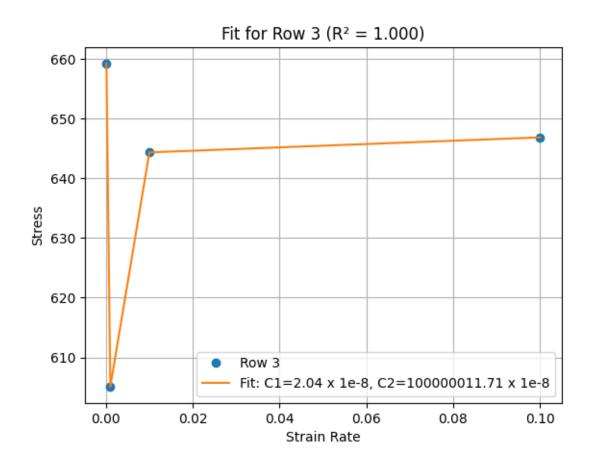


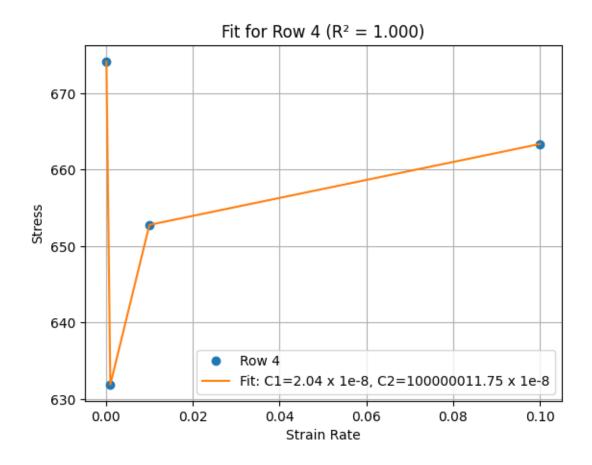


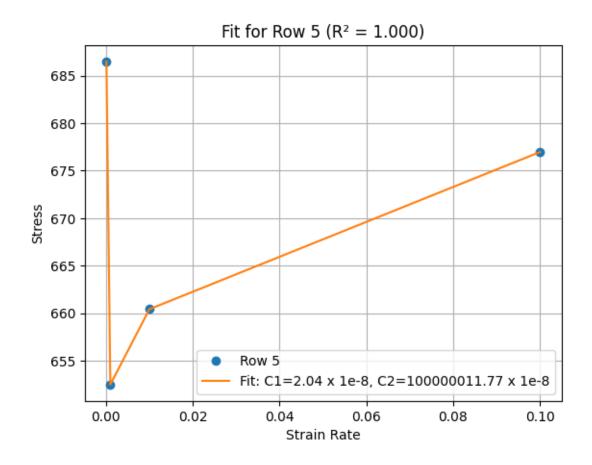


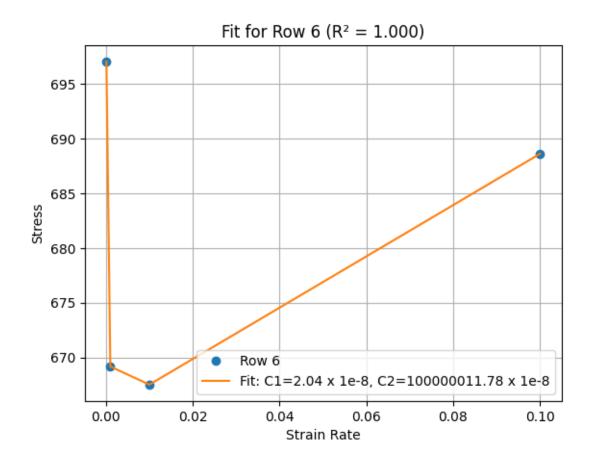


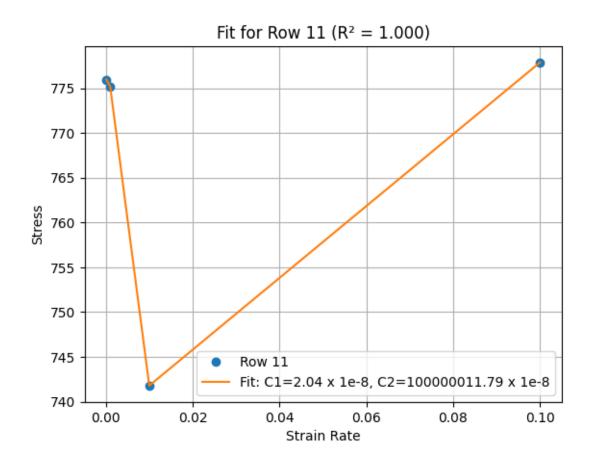
## 2.2 Other cases

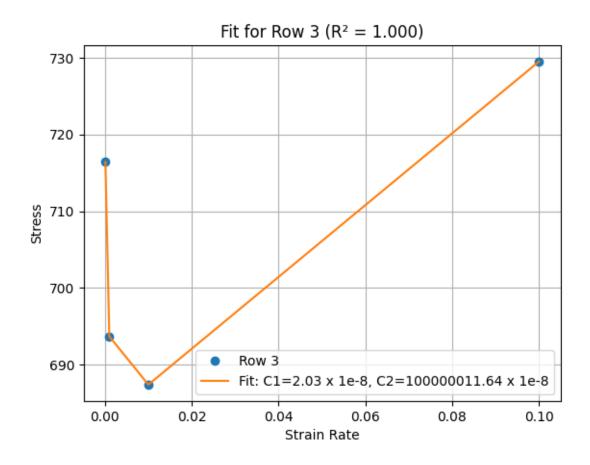


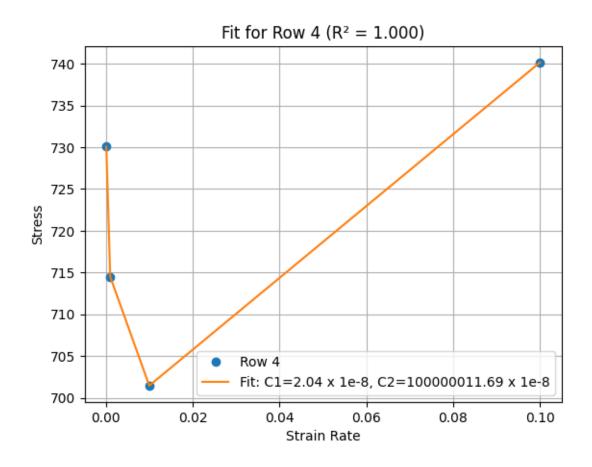


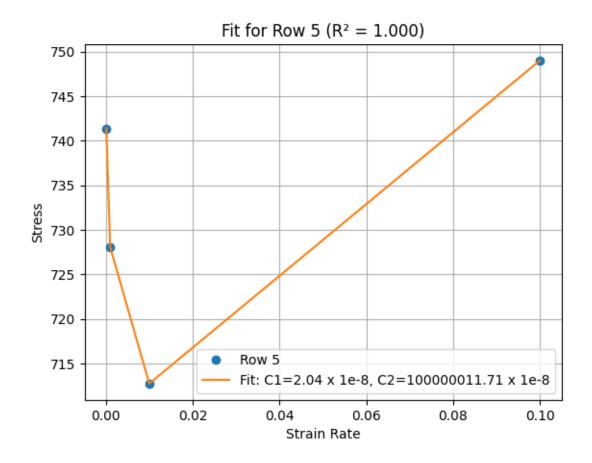


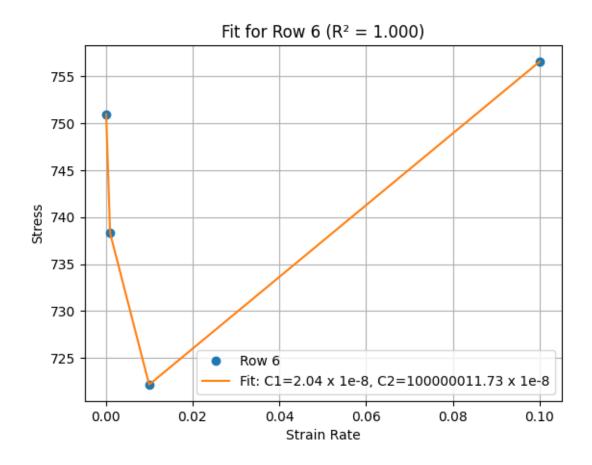


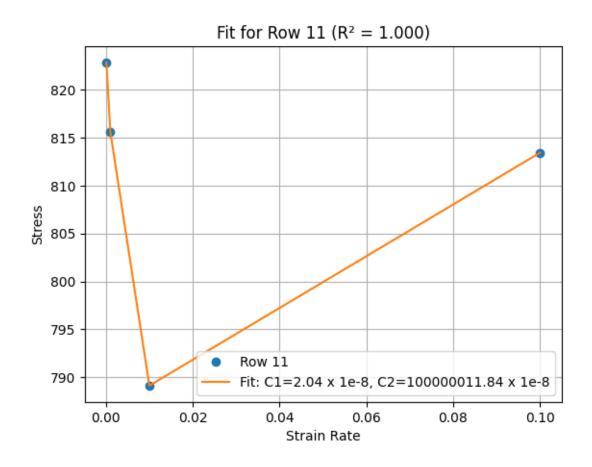


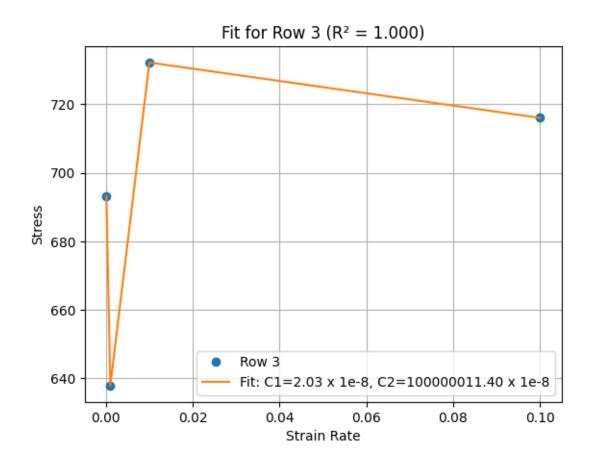


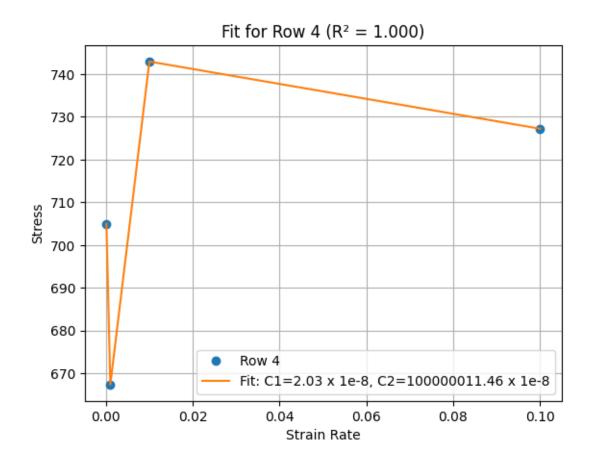


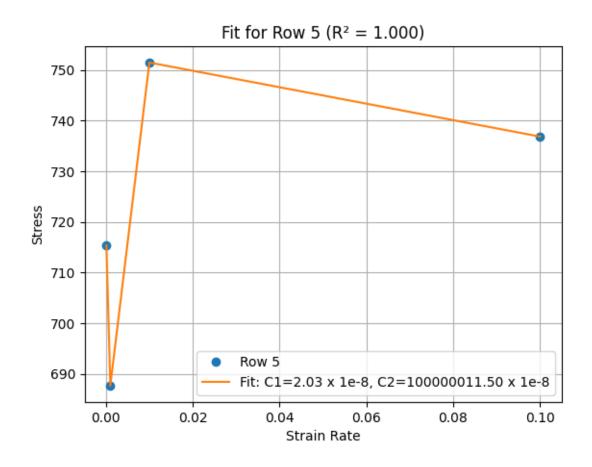


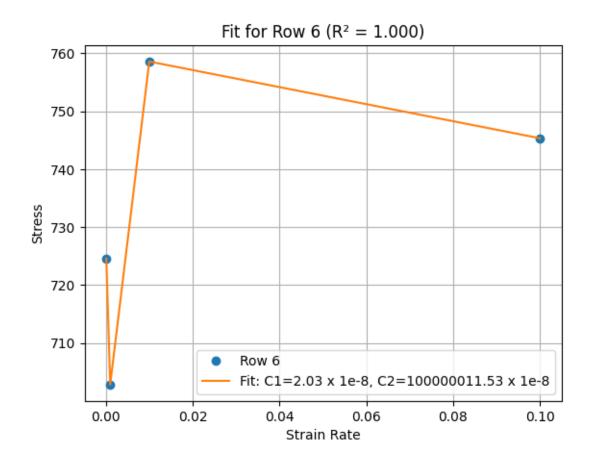


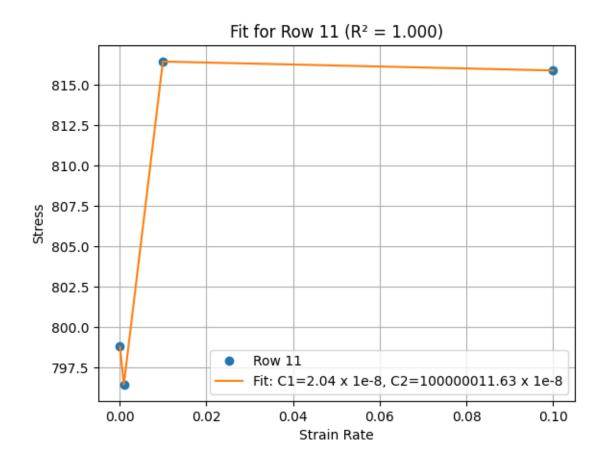


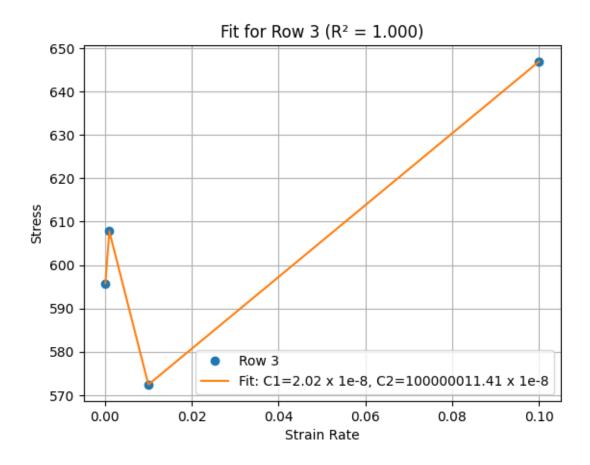


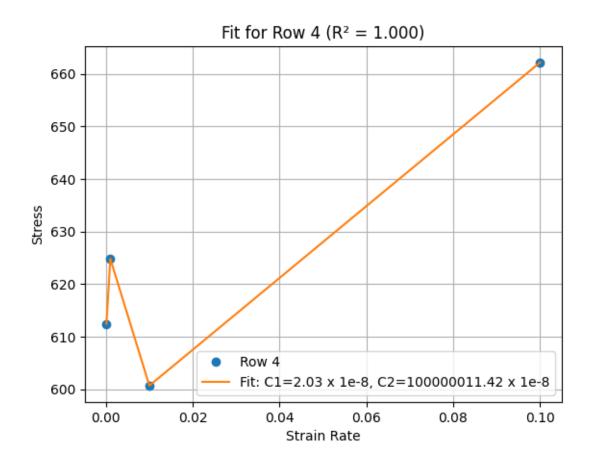


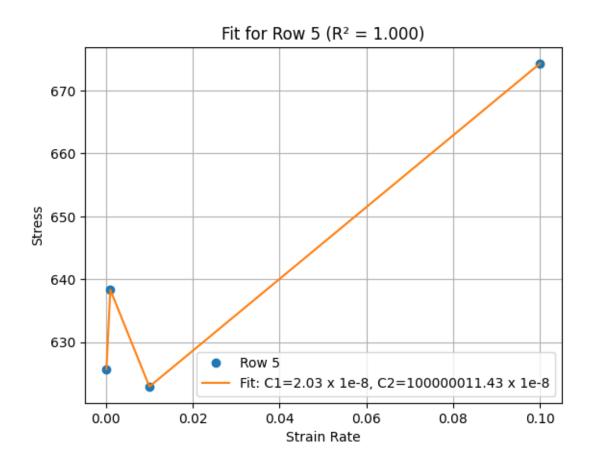


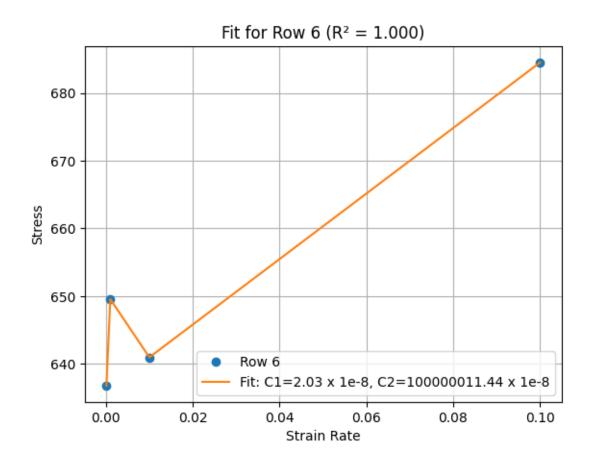


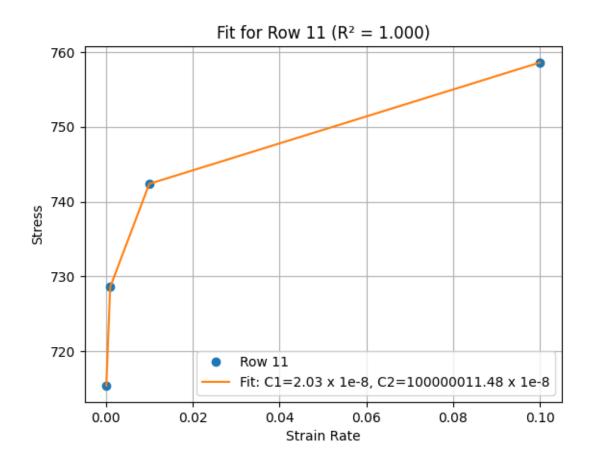












## 3 Check R1 score

#### 3.1 Check to see if any R1 < 0.998

```
[]: def check_r_squared(temperature_files):
    """
    Checks R_squared values in the Parameters file for each temperature and preports any below 0.99.

Parameters:
    - temperature_files (list of str): List of temperature file names (without process):
    "".csv" extension).

Output:
    - Prints any rows with R_squared < threshold for each temperature file.
    """

threshold = 0.999
    for temp_file in temperature_files:
        # Load the data from the CSV file
```

```
df = pd.read_csv(f"Parameters_{temp_file}.csv")

# Filter rows where R_squared is less than 0.99
low_r_squared = df[df['R_squared'] < threshold]

if not low_r_squared.empty:
    print(f"\nTemperature File: Parameters_{temp_file}.csv")
    print(f"Rows with R_squared < {threshold}:")
    print(low_r_squared[['PEEQ', 'C1', 'C2', 'R_squared']])
else:
    print(f"\nTemperature File: Parameters_{temp_file}.csv")
    print(f"All R_squared values are >= {threshold}.")

#Usage
temperature_files = ['Tmp298.15_RD', 'Tmp373.15_RD', 'Tmp473.15_RD', 'Tmp573.
    \( \to 15_RD', 'Tmp673.15_RD'] \) # List of temperature files to check
check_r_squared(temperature_files)
```

```
Temperature File: Parameters_Tmp298.15_RD.csv
All R_squared values are >= 0.999.

Temperature File: Parameters_Tmp373.15_RD.csv
All R_squared values are >= 0.999.

Temperature File: Parameters_Tmp473.15_RD.csv
All R_squared values are >= 0.999.

Temperature File: Parameters_Tmp573.15_RD.csv
All R_squared values are >= 0.999.

Temperature File: Parameters_Tmp673.15_RD.csv
All R_squared values are >= 0.999.
```

# 4 Calibrate C1, C2 based on strain dependent

### 4.1 Study relationship between C1, C2

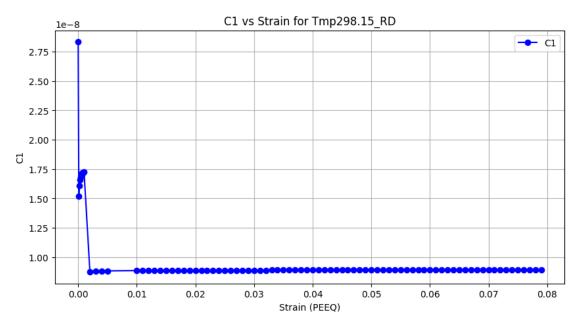
C1, C2 follows the same trend for a condition and is dependent on strain rate => Use the same strain dependent function

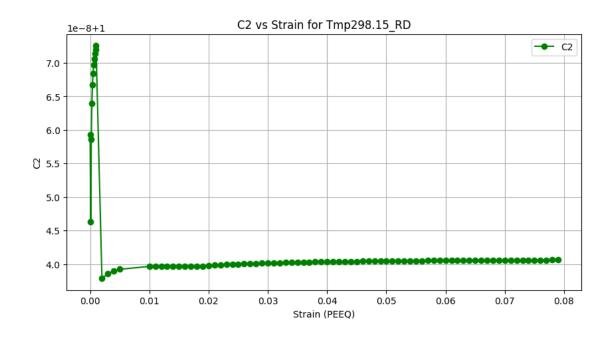
```
[]: # List of temperature files to load
temperature_files = ['Tmp298.15_RD', 'Tmp373.15_RD', 'Tmp473.15_RD', 'Tmp573.

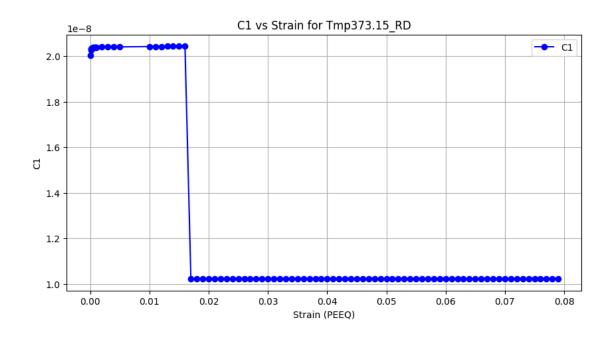
→15_RD', 'Tmp673.15_RD']

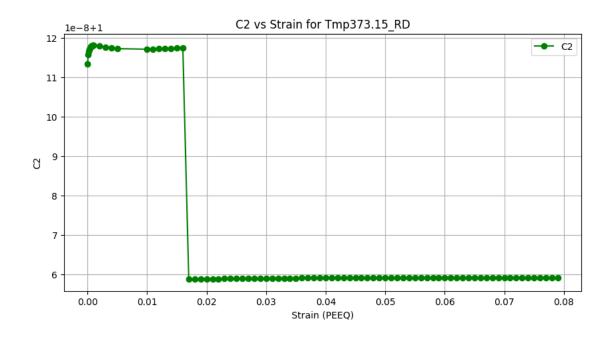
# Loop through each temperature file and plot C1 and C2 against strain (PEEQ)
for temp_file in temperature_files:
```

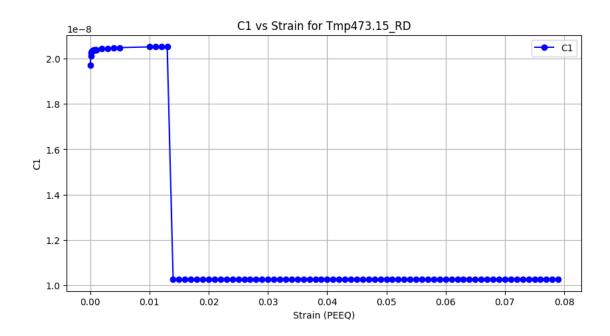
```
# Load the data from the CSV file
  df = pd.read_csv(f"Parameters_{temp_file}.csv")
  # Plot C1 vs. strain with lines
  plt.figure(figsize=(10, 5))
  plt.plot(df['PEEQ'], df['C1'], marker='o', color='blue', label='C1') #__
→Line plot with points
  plt.xlabel('Strain (PEEQ)')
  plt.ylabel('C1')
  plt.title(f"C1 vs Strain for {temp_file}")
  plt.legend()
  plt.grid()
  plt.show()
  # Plot C2 vs. strain with lines
  plt.figure(figsize=(10, 5))
  plt.plot(df['PEEQ'], df['C2'], marker='o', color='green', label='C2') #__
→Line plot with points
  plt.xlabel('Strain (PEEQ)')
  plt.ylabel('C2')
  plt.title(f"C2 vs Strain for {temp_file}")
  plt.legend()
  plt.grid()
  plt.show()
```

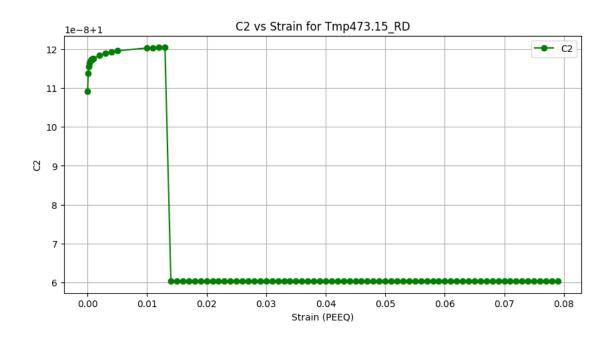


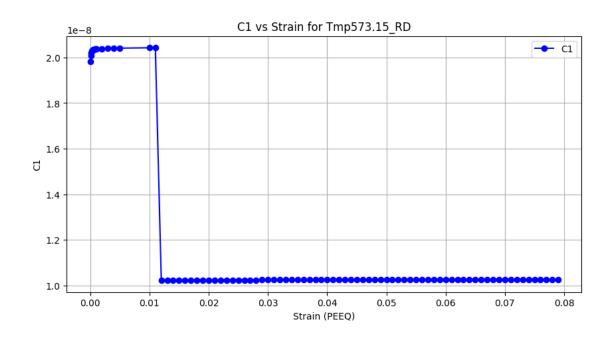


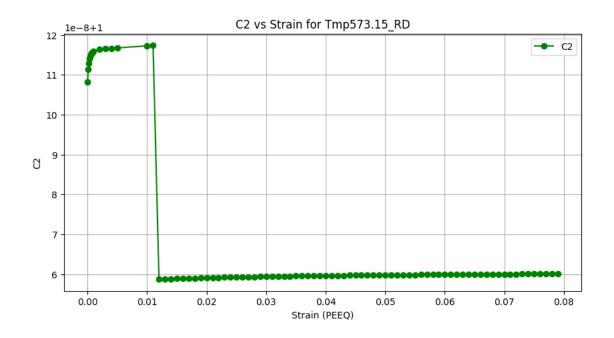


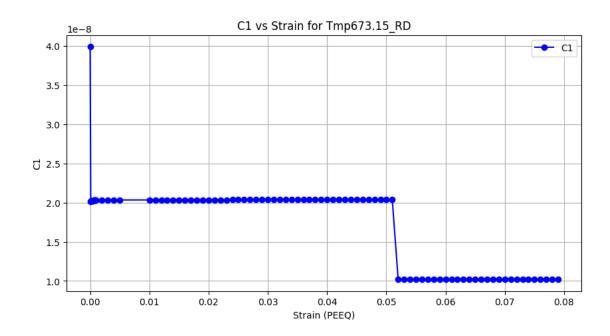


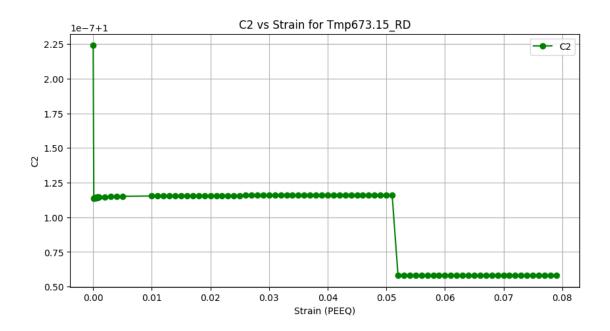












#### 4.2 Calibrate strain dependent function for C1 and C2

```
[]: def calibrate_strain_dependent(temp_file):
        data = pd.read_csv(f"Parameters_{temp_file}.csv") # Replace with your_
      ⇔actual file path
         strain = data['PEEQ'] # Strain values
        C1_values = data['C1'] # C1 values
        C2_values = data['C2'] # C2 values
         # Define the stretched exponential model
        def stretched_exponential(epsilon, a, b, c, d):
            return a * np.exp(-b * epsilon**c) + d
         # Initial guesses for C1
         initial_guess_C1 = [2.0, 10, 0.5, 0.9]
         # Fit the stretched exponential model to C1
        popt_C1, _ = curve_fit(stretched_exponential, strain, C1_values,__
      →p0=initial_guess_C1, maxfev=10000000)
         # Generate strain values for fitting curves
        strain_fit = np.linspace(min(strain), max(strain), 100)
         # Grid search for the best initial guess for C2 parameters
         # Define small ranges around a reasonable starting point for each parameter
        a_range = np.linspace(1.0, 3.0, 10)
                                                # Wider range for a
```

```
b_range = np.linspace(5, 15, 10)  # Wider range for b
c_range = np.linspace(0.3, 0.7, 10)  # Wider range for c
d_range = np.linspace(0.8, 1.2, 10)  # Wider range for d
   best_params_C2 = None
   best_r2_C2 = -np.inf
   # Perform grid search over the parameter ranges
   for a, b, c, d in product(a_range, b_range, c_range, d_range):
       try:
            popt_C2, _ = curve_fit(stretched_exponential, strain, C2_values,__
\Rightarrowp0=[a, b, c, d], maxfev=10000000)
           C2_fitted_values = stretched_exponential(strain, *popt_C2)
           r2_C2 = r2_score(C2_values, C2_fitted_values)
            if r2_C2 > best_r2_C2:
                best_r2_C2 = r2_C2
                best_params_C2 = popt_C2
       except RuntimeError:
            continue
   # Use the best parameters found for C2
   popt_C2 = best_params_C2
   # Generate fitted values using the stretched exponential model
   C1_fit = stretched_exponential(strain_fit, *popt_C1)
   C2_fit = stretched_exponential(strain_fit, *popt_C2)
   # Calculate the fitted values at the original strain points for R^2 score_
\hookrightarrow calculation
   C1_fitted_values = stretched_exponential(strain, *popt_C1)
   C2_fitted_values = stretched_exponential(strain, *popt_C2)
   # Calculate R^2 scores
   r2 C1 = r2 score(C1 values, C1 fitted values)
   # Plot C1 vs Strain with stretched exponential fit
   plt.figure(figsize=(10, 5))
   plt.plot(strain, C1_values, 'o', label='C1 Data')
   plt.plot(strain_fit, C1_fit, '-', label='C1 Fit (Stretched Exponential)')
   plt.xlabel('Strain (PEEQ)')
   plt.ylabel('C1')
   plt.legend()
   plt.title(f"C1 vs Strain with Stretched Exponential Fit {temp_file} (R^2:
\hookrightarrow{r2_C1:.3f})")
   plt.show()
   plt.savefig(f"results/C1_{temp_file}.png")
```

```
# Plot C2 vs Strain with stretched exponential fit
   plt.figure(figsize=(10, 5))
   plt.plot(strain, C2_values, 'o', label='C2 Data')
   plt.plot(strain_fit, C2_fit, '-', label='C2 Fit (Stretched Exponential)')
   plt.xlabel('Strain (PEEQ)')
   plt.ylabel('C2')
   plt.legend()
   plt.title(f"C2 vs Strain with Stretched Exponential Fit {temp_file} (R^2:__
 \rightarrow{best_r2_C2:.3f})")
   plt.savefig(f"results/C2_{temp_file}.png")
   plt.show()
    # Print the fitted parameters for reference
   print("Stretched Exponential Fit Parameters for C1:", popt_C1)
   print("Best Stretched Exponential Fit Parameters for C2:", best_params_C2)
   print("Best R^2 for C2:", best_r2_C2)
# Example usage:
# calibrate strain dependent('Tmp673.15 RD')
```

```
[]: temperature_files = ['Tmp298.15_RD', 'Tmp373.15_RD', 'Tmp473.15_RD', 'Tmp573.

□15_RD', 'Tmp673.15_RD']

# Loop through each temperature file and plot C1 and C2 against strain (PEEQ)
for temp_file in temperature_files:
    calibrate_strain_dependent(temp_file)
```

/Library/Frameworks/Python.framework/Versions/3.11/lib/python3.11/site-packages/scipy/optimize/\_minpack\_py.py:906: OptimizeWarning: Covariance of the parameters could not be estimated

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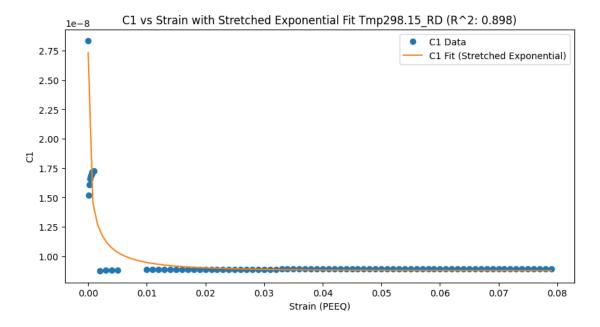
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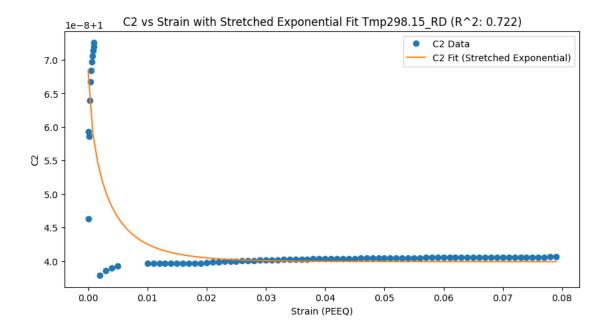
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Stretched Exponential Fit Parameters for C1: [1.85478856e-08 2.14878456e+01 4.08332239e-01 8.76551457e-09]

Best Stretched Exponential Fit Parameters for C2: [2.85599188e-08 6.33748493e+01 7.11482800e-01 1.00000004e+00]

Best R^2 for C2: 0.7222662006658567

/Library/Frameworks/Python.framework/Versions/3.11/lib/python3.11/site-packages/scipy/optimize/\_minpack\_py.py:486: RuntimeWarning: overflow encountered in matmul

cov\_x = invR @ invR.T

/Library/Frameworks/Python.framework/Versions/3.11/lib/python3.11/site-packages/scipy/optimize/\_minpack\_py.py:906: OptimizeWarning: Covariance of the parameters could not be estimated

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warnings.warn('Covariance of the parameters could not be estimated', /Users/linh/Library/Python/3.11/lib/python/site-packages/pandas/core/arraylike.py:396: RuntimeWarning: overflow encountered in exp

result = getattr(ufunc, method)(\*inputs, \*\*kwargs)
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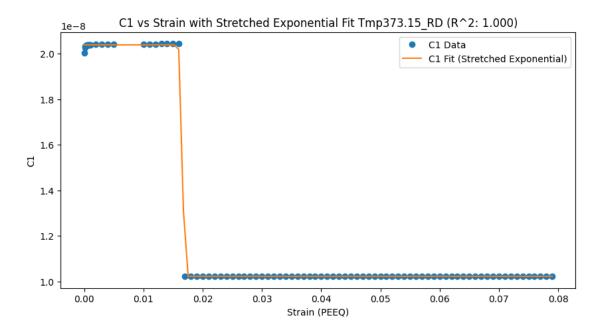
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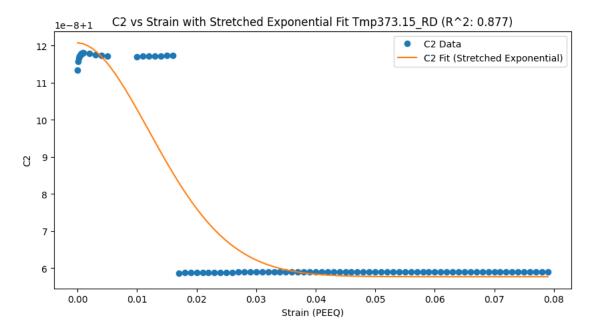
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Stretched Exponential Fit Parameters for C1: [1.01733286e-008 1.19861793e+152 8.55811948e+001 1.02176444e-008]

Best Stretched Exponential Fit Parameters for C2: [6.30589591e-08 1.90697795e+03 1.87720219e+00 1.00000006e+00]

Best R^2 for C2: 0.8766807063588724

/Library/Frameworks/Python.framework/Versions/3.11/lib/python3.11/site-packages/scipy/optimize/\_minpack\_py.py:486: RuntimeWarning: overflow encountered in matmul

cov\_x = invR @ invR.T

/Library/Frameworks/Python.framework/Versions/3.11/lib/python3.11/site-packages/scipy/optimize/\_minpack\_py.py:906: OptimizeWarning: Covariance of the parameters could not be estimated

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warnings.warn('Covariance of the parameters could not be estimated', /Users/linh/Library/Python/3.11/lib/python/site-packages/pandas/core/arraylike.py:396: RuntimeWarning: overflow encountered in exp

result = getattr(ufunc, method)(\*inputs, \*\*kwargs)
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warnings.warn('Covariance of the parameters could not be estimated', /Users/linh/Library/Python/3.11/lib/python/site-packages/pandas/core/arraylike.py:396: RuntimeWarning: overflow encountered in exp

result = getattr(ufunc, method)(\*inputs, \*\*kwargs)

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packages/pandas/core/arraylike.py:396: RuntimeWarning: overflow encountered in exp

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warnings.warn('Covariance of the parameters could not be estimated', /Users/linh/Library/Python/3.11/lib/python/site-

packages/pandas/core/arraylike.py:396: RuntimeWarning: overflow encountered in exp

result = getattr(ufunc, method)(\*inputs, \*\*kwargs)
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warnings.warn('Covariance of the parameters could not be estimated', /Users/linh/Library/Python/3.11/lib/python/site-packages/pandas/core/arraylike.py:396: RuntimeWarning: overflow encountered in exp

result = getattr(ufunc, method)(\*inputs, \*\*kwargs)
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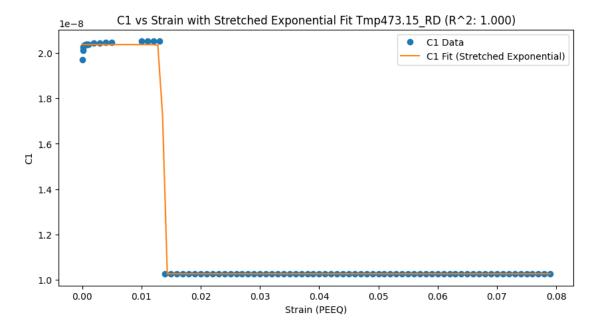
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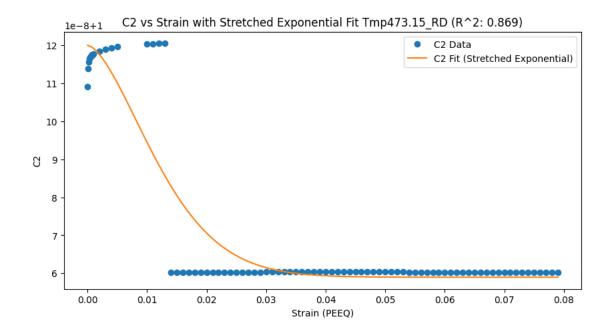
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Stretched Exponential Fit Parameters for C1: [1.01130864e-008 1.11507528e+152 8.16476951e+001 1.02609960e-008]

Best Stretched Exponential Fit Parameters for C2: [6.10290280e-08 9.08802029e+02 1.61192759e+00 1.00000006e+00]

Best R^2 for C2: 0.8688254701508767

/Library/Frameworks/Python.framework/Versions/3.11/lib/python3.11/site-packages/scipy/optimize/\_minpack\_py.py:906: OptimizeWarning: Covariance of the parameters could not be estimated

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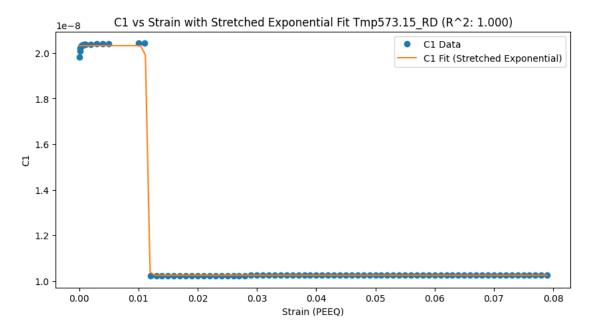
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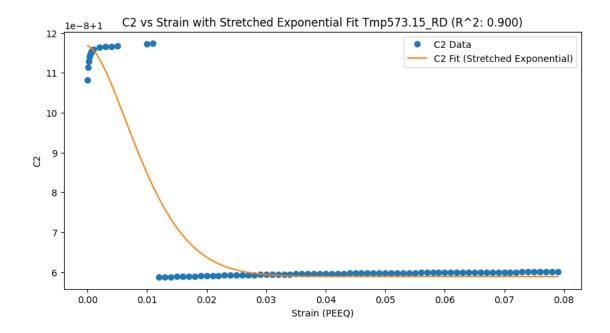
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Stretched Exponential Fit Parameters for C1: [1.00759288e-008 2.75751813e+129 6.70220191e+001 1.02459104e-008]

Best Stretched Exponential Fit Parameters for C2: [5.79176500e-08 1.39167746e+03 1.61824434e+00 1.00000006e+00]

Best R^2 for C2: 0.8997917516929005

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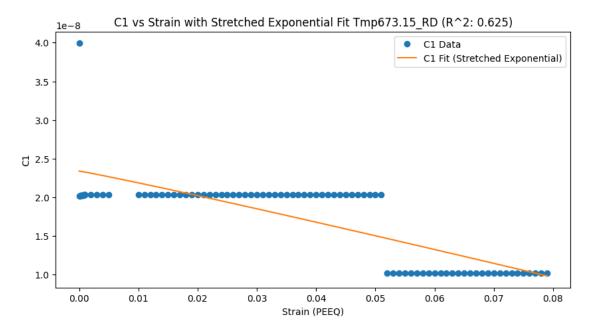
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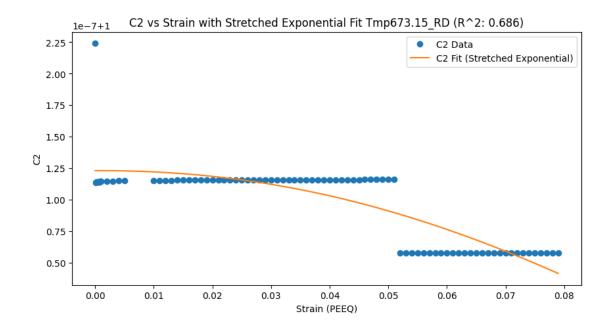
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Stretched Exponential Fit Parameters for C1: [ 3.14248936e-02 6.29880084e-06 1.05611275e+00 -3.14248702e-02]

Best Stretched Exponential Fit Parameters for C2: [5.94436324e-07 3.44949406e+01 2.14876129e+00 9.99999529e-01]

Best R^2 for C2: 0.6859290526332873

## 5 Bonus

Temperature dependence and normalized stress

```
[]:
    ref_temp = '298.15'

#First set, comment out second set to generate for this one
    strain_rates = [0.0001]
    temps = ['77.15', '233.15', '298.15', '373.15', '473.15', '573.15', '673.15']

#Second set
    strain_rates = [0.001, 0.01, 0.1]
    temps = ['298.15', '373.15', '473.15', '573.15', '673.15']

for strain_rate in strain_rates:
    # Load reference stress data at 298.15 K for the given strain rate
    data_RD_ref = pd.read_csv(f'../extended_curve/
    \[
Tmp{ref_temp}K_StrRt{strain_rate}_RD.csv')
    ref_stress_RD = data_RD_ref['Stress'] # Stress column at reference_
    \[
\int temperature
```

```
# Initialize DataFrame with strain column
    df = pd.DataFrame({'strain': data_RD_ref['Strain']})
    # Loop over each temperature to calculate and add normalized stress columns
    for temp in temps:
        # Load stress data at the current temperature
        temp_RD = pd.read_csv(f'../extended_curve/
 \neg Tmp\{temp\}K\_StrRt\{strain\_rate\}\_RD.csv')['Stress']
        # Calculate normalized stress by dividing by reference stress at 298.15_{\sqcup}
 \hookrightarrow K
        normalized_stress_RD = temp_RD / ref_stress_RD
        # Add normalized stress as a column in the DataFrame
        df[f'Tmp{temp}K_ref'] = normalized_stress_RD
    # Save the DataFrame to a CSV file
    df = df[df['strain'] < 0.08]
    output_file_path = f"StrainRate{strain_rate}_RD.csv"
    df.to_csv(output_file_path, index=False)
,,,
I I I
def organise_data_normalized(strain_rates, temps):
    ref_temp = '298.15'
    # Loop over each temperature
    for temp in temps:
        df = None # Initialize df to None to handle it dynamically for each \Box
 \hookrightarrow temperature
        for strain_rate in strain_rates:
            # Load reference stress data at 298.15 K for the given strain rate
            data_RD_ref = pd.read_csv(f'../extended_curve/
 → Tmp{ref_temp}K_StrRt{strain_rate}_RD.csv')
            ref_stress_RD = data_RD_ref['Stress']
            # Load current temperature stress data for the given strain rate
            data_RD = pd.read_csv(f'../extended_curve/
 \neg Tmp\{temp\}K\_StrRt\{strain\_rate\}\_RD.csv'\}
            # Calculate normalized stress
            normalized_stress_RD = data_RD['Stress'] / ref_stress_RD
            if df is None:
                 # Initialize DataFrame with strain column if not already done
```

```
df = pd.DataFrame({'strain': data_RD['Strain']})

# Add normalized stress data for the current strain rate as a new_
column

df[f'StrRt{strain_rate}'] = normalized_stress_RD

# Filter the DataFrame for strain values below 0.08

df = df[df['strain'] < 0.08]

# Save the DataFrame to a CSV file for the current temperature output_file_path = f"Tmp{temp}_RD_normalized.csv"

df.to_csv(output_file_path, index=False)

'''</pre>
```

```
[]: '\ndef organise data normalized(strain rates, temps):\n
                                                               ref temp =
    \'298.15\'\n\n
                          # Loop over each temperature\n
                                                            for temp in temps:\n
    df = None # Initialize df to None to handle it dynamically for each
    temperature\n
                                   for strain rate in strain rates:\n
                         \n
    Load reference stress data at 298.15 K for the given strain rate\n
    data RD ref =
    pd.read_csv(f\'../extended_curve/Tmp{ref_temp}K_StrRt{strain_rate}_RD.csv\')\n
    ref_stress_RD = data_RD_ref[\'Stress\']\n
                                                         \n
                                                                       # Load
    current temperature stress data for the given strain rate\n
                                                                           data_RD =
    pd.read_csv(f\'../extended_curve/Tmp{temp}K StrRt{strain_rate}_RD.csv\')\n
    \n
                  # Calculate normalized stress\n
                                                             normalized_stress_RD =
    data RD[\'Stress\'] / ref stress RD\n
                                                                   if df is None:\n
    # Initialize DataFrame with strain column if not already done\n
    df = pd.DataFrame({\'strain\': data RD[\'Strain\']})\n
    # Add normalized stress data for the current strain rate as a new column\n
    df[f\'StrRt{strain_rate}\'] = normalized_stress_RD\n\n
                                                                  # Filter the
    DataFrame for strain values below 0.08\n
                                                    df = df[df[\train'] < 0.08]\n
              # Save the DataFrame to a CSV file for the current temperature\n
    output file path = f"Tmp{temp} RD normalized.csv"\n
    df.to_csv(output_file_path, index=False)\n'
```