sv_fitting

September 25, 2024

[ ]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from scipy.optimize import curve_fit
from matplotlib.backends.backend_pdf import PdfPages
```

1 Normal Swift-Voce fitting

[ ]:
```
def analyze_sv_fit(file_path, strain_column, stress_column, title,␣
 ↪initial_guess=None):
# Load data in
    data = pd.read_csv(file_path)
    strain = data[strain_column].dropna().values
    stress = data[stress_column].dropna().values

# Define the Swift-Voce equation
    def swift_voce(strain, alpha, A, epsilon_0, n, k0, Q, beta):
        swift_term = alpha * A * (epsilon_0 + strain) ** n
        voce_term = (1 - alpha) * (k0 + Q * (1 - np.exp(-beta * strain)))
        return swift_term + voce_term

# Initial guesses for parameters [alpha, A, epsilon_0, n, k0, Q, beta]
    initial_guess = [0.5, 500, 0.01, 0.2, 300, 200, 10]

# Fit the curve
    params, _ = curve_fit(swift_voce, strain, stress, p0=initial_guess,␣
 ↪maxfev=20000)

# Extract fitted parameters
    alpha, A, epsilon_0, n, k0, Q, beta = params

# Plot the experimental data and the fitted curve
    fitted_stress = swift_voce(strain, *params)
    plt.scatter(strain, stress, label='Experimental Data', color='red')
    plt.plot(strain, fitted_stress, label='Fitted Curve', color='blue')
    plt.xlabel('True Strain')
    plt.ylabel('True Stress')
```

```
    plt.title(title)
    plt.legend()
    plt.show()

# Print fitted parameters
    print(f'Fitted Parameters:\nAlpha: {alpha:.4f}\nA: {A:.4f}\nEpsilon_0:␣
↪{epsilon_0:.4f}\n'
      f'n: {n:.4f}\nK0: {k0:.4f}\nQ: {Q:.4f}\nBeta: {beta:.4f}\n')

# Calculate error metrics
    mse = np.mean((stress - fitted_stress) ** 2)
    rmse = np.sqrt(mse)
    mae = np.mean(np.abs(stress - fitted_stress))
    r_squared = 1 - np.sum((stress - fitted_stress) ** 2) / np.sum((stress - np.
↪mean(stress)) ** 2)

    # Print error metrics
    print(f'Error Metrics:\n'
          f'MSE: {mse:.4f}\n'
          f'RMSE: {rmse:.4f}\n'
          f'MAE: {mae:.4f}\n'
          f'R-squared: {r_squared:.4f}')

# Extended strain for comparison (you might want to adjust this range)
    extended_strain = np.concatenate((strain, np.arange(strain[-1] + 0.01, 2.
↪01, 0.01)))
    extended_stress = swift_voce(extended_strain, *params)
    plt.scatter(strain, stress, label='Experimental Data', color='red')
    plt.plot(extended_strain, extended_stress, label='Fitted Curve',␣
↪color='blue')
    plt.xlabel('True Strain')
    plt.ylabel('True Stress')
    plt.title(f"{title}_extended")
    plt.legend()
    plt.show()

    '''
    # Export stress and strain values
    stress_difference = stress - fitted_stress

    # Create a DataFrame with the required columns
    df = pd.DataFrame({
        'Experimental Strain': strain,
        'Experimental Stress': stress,
        'Fitted Stress': fitted_stress,
        'Stress Difference': stress_difference
    })
```

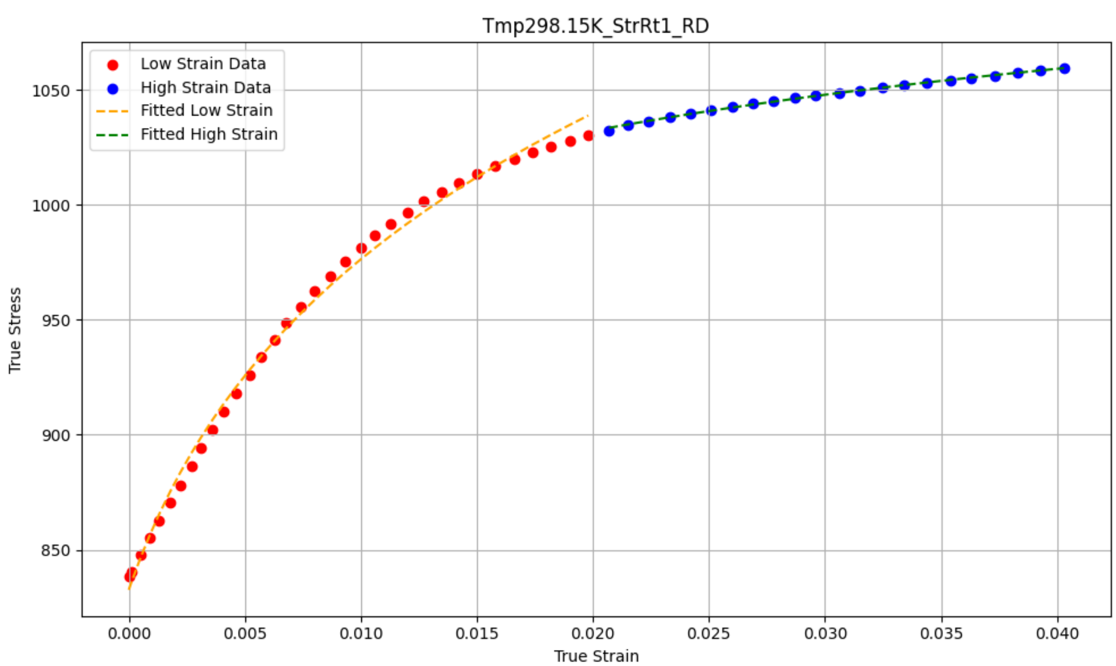
```
    extracted_strain = np.arange(0.1, 3.01, 0.01)
    extracted_stress = swift_voce(extracted_strain, *params)
    df2 = pd.DataFrame({
        'Extended Strain': extracted_strain,
        'Extended Stress': extracted_stress,
    })

    # Save the DataFrame to an Excel file with the file name based on the␣
↪`title` argument
    output_file_path = f"{title}_stress_strain_comparison.xlsx"
    with pd.ExcelWriter(output_file_path) as writer:
        df.to_excel(writer, sheet_name='Comparison', index=False)
        df2.to_excel(writer, sheet_name='Extended Fit', index=False)

    print(f"Data has been exported to {output_file_path}")
    '''
    return params
```

2 Modified Swift-Voce fitting with damping value for high strain

```
[ ]: def analyze_msv_fit(file_path, strain_column, stress_column, title,␣
↪initial_guess=None):
    # Load data
    data = pd.read_csv(file_path)
    strain = data[strain_column].dropna().values
    stress = data[stress_column].dropna().values

    # Define the Modified Swift-Voce equation
    def modified_swift_voce(strain, A, B, n, K, epsilon0, alpha, beta):
        swift_part = A * (strain + epsilon0) ** n  # Swift law
        voce_part = K * (1 - np.exp(-B * strain))  # Voce law
        damping = (1 - np.exp(-alpha * strain)) / (1 + beta * strain)  #␣
↪Damping term
        return swift_part + voce_part * damping

    # Initial guesses for parameters [A, B, n, K, epsilon0, alpha, beta]
    if initial_guess is None:
        initial_guess = [1500, 20, 0.2, 2000, 0.02, 0.3, 5] # Default values if␣
↪not provided

    # Adjusted bounds to limit parameter values
    bounds = ([500, 0, 0, 500, 0, 0, 0], [5000, 50, 1, 5000, 0.2, 1, 20])

    # Separate data into low and high strain regions
    low_strain = strain[strain < 0.02]
```

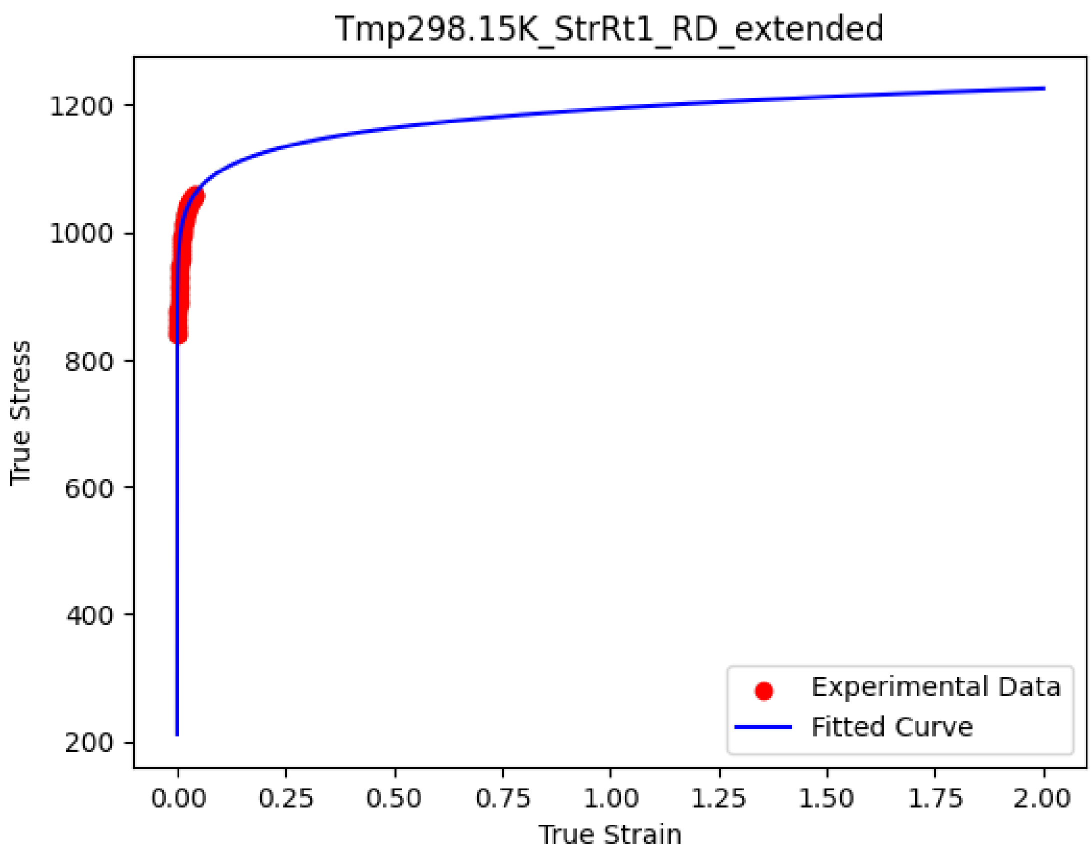
```
    low_stress = stress[strain < 0.02]

    high_strain = strain[strain >= 0.02]
    high_stress = stress[strain >= 0.02]

    # Fit the curve for low strain data
    params_low, _ = curve_fit(
        modified_swift_voce, low_strain, low_stress, p0=initial_guess,␣
↪bounds=bounds
    )

    # Fit the curve for high strain data
    params_high, _ = curve_fit(
        modified_swift_voce, high_strain, high_stress, p0=initial_guess,␣
↪bounds=bounds
    )

    # Extract fitted stress values
    fitted_low_stress = modified_swift_voce(low_strain, *params_low)
    fitted_high_stress = modified_swift_voce(high_strain, *params_high)

    # Plot experimental and fitted curves
    plt.figure(figsize=(10, 6))
    plt.scatter(low_strain, low_stress, label='Low Strain Data', color='red')
    plt.scatter(high_strain, high_stress, label='High Strain Data',␣
↪color='blue')
    plt.plot(low_strain, fitted_low_stress, color='orange', linestyle='--',␣
↪label='Fitted Low Strain')
    plt.plot(high_strain, fitted_high_stress, color='green', linestyle='--',␣
↪label='Fitted High Strain')

    plt.xlabel('True Strain')
    plt.ylabel('True Stress')
    plt.title(title)
    plt.legend()
    plt.grid(True)
    plt.tight_layout()
    plt.show()

    # Print fitted parameters for both regions
    print(f'Fitted Parameters for Low Strain (<0.02):\n'
          f'A: {params_low[0]:.4f}, B: {params_low[1]:.4f}, n: {params_low[2]:.
↪4f}, '
          f'K: {params_low[3]:.4f}, Epsilon_0: {params_low[4]:.4f}, '
          f'Alpha: {params_low[5]:.4f}, Beta: {params_low[6]:.4f}')
```

```
    print(f'Fitted Parameters for High Strain (>=0.02):\n'
          f'A: {params_high[0]:.4f}, B: {params_high[1]:.4f}, n:␣
 ↪{params_high[2]:.4f}, '
          f'K: {params_high[3]:.4f}, Epsilon_0: {params_high[4]:.4f}, '
          f'Alpha: {params_high[5]:.4f}, Beta: {params_high[6]:.4f}')

    extended_strain = np.concatenate((strain, np.arange(strain[-1] + 0.01, 2.
 ↪01, 0.01)))
    extended_stress = modified_swift_voce(extended_strain, *params_high)
    plt.scatter(strain, stress, label='Experimental Data', color='red')
    plt.plot(extended_strain, extended_stress, label='Fitted Curve',␣
 ↪color='blue')
    plt.xlabel('True Strain')
    plt.ylabel('True Stress')
    plt.title(f"{title}_extended")
    plt.legend()
    plt.show()

    return params_low, params_high

condition = 'Tmp298.15K_StrRt1_RD'
analyze_msv_fit('data/Exp_FC_StrRtDpn_TmpDpn_Tmp298.csv', condition + '_E',␣
 ↪condition + '_S', condition)
```




```
Fitted Parameters for Low Strain (<0.02):
```

```
A: 1581.8136, B: 18.7997, n: 0.1114, K: 1891.1069, Epsilon_0: 0.0031, Alpha:
0.0000, Beta: 19.9786
Fitted Parameters for High Strain (>=0.02):
A: 1194.0092, B: 14.7818, n: 0.0373, K: 759.6380, Epsilon_0: 0.0000, Alpha:
0.0000, Beta: 6.3350
```



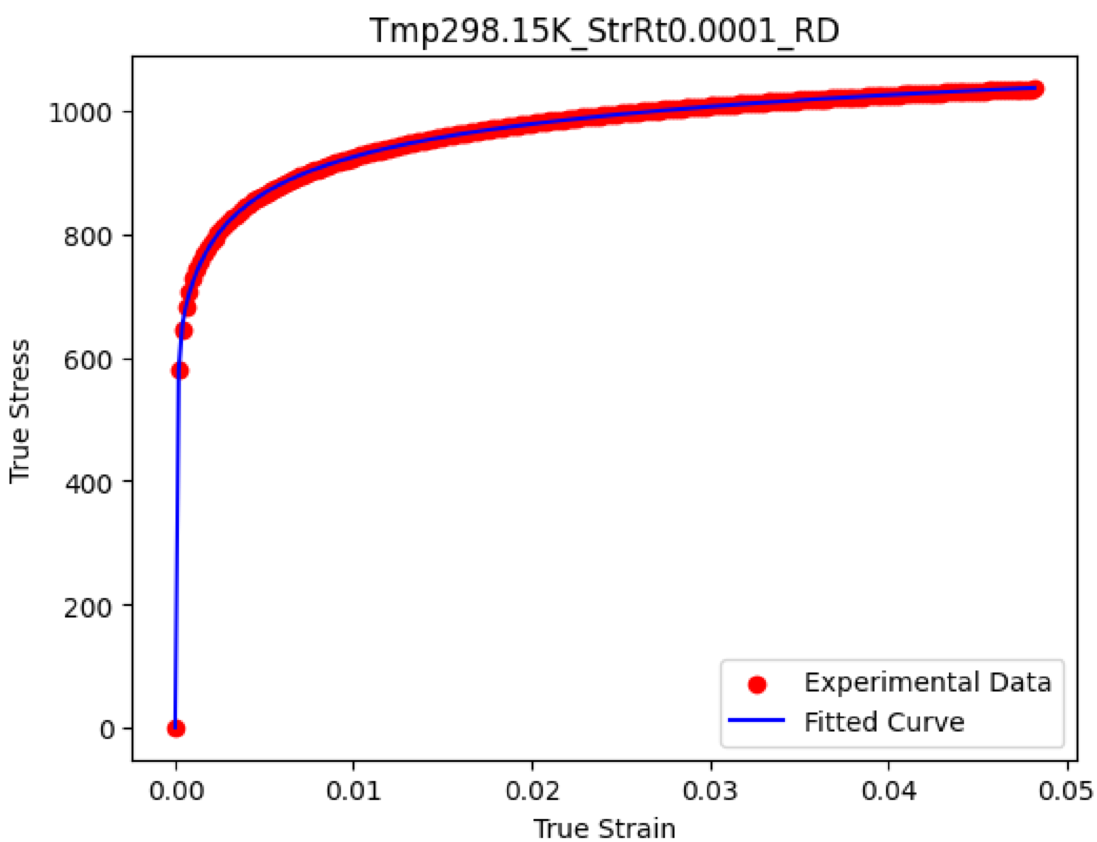
[ ]:
```
(array([1.58181360e+03, 1.87997462e+01, 1.11411675e-01, 1.89110690e+03,
        3.14836951e-03, 7.70761622e-13, 1.99786230e+01]),
 array([1.19400920e+03, 1.47817668e+01, 3.72508750e-02, 7.59638004e+02,
        6.16173973e-21, 6.07998938e-30, 6.33500171e+00]))
```

3 Plot of all strain rate at RT and parameters relationship

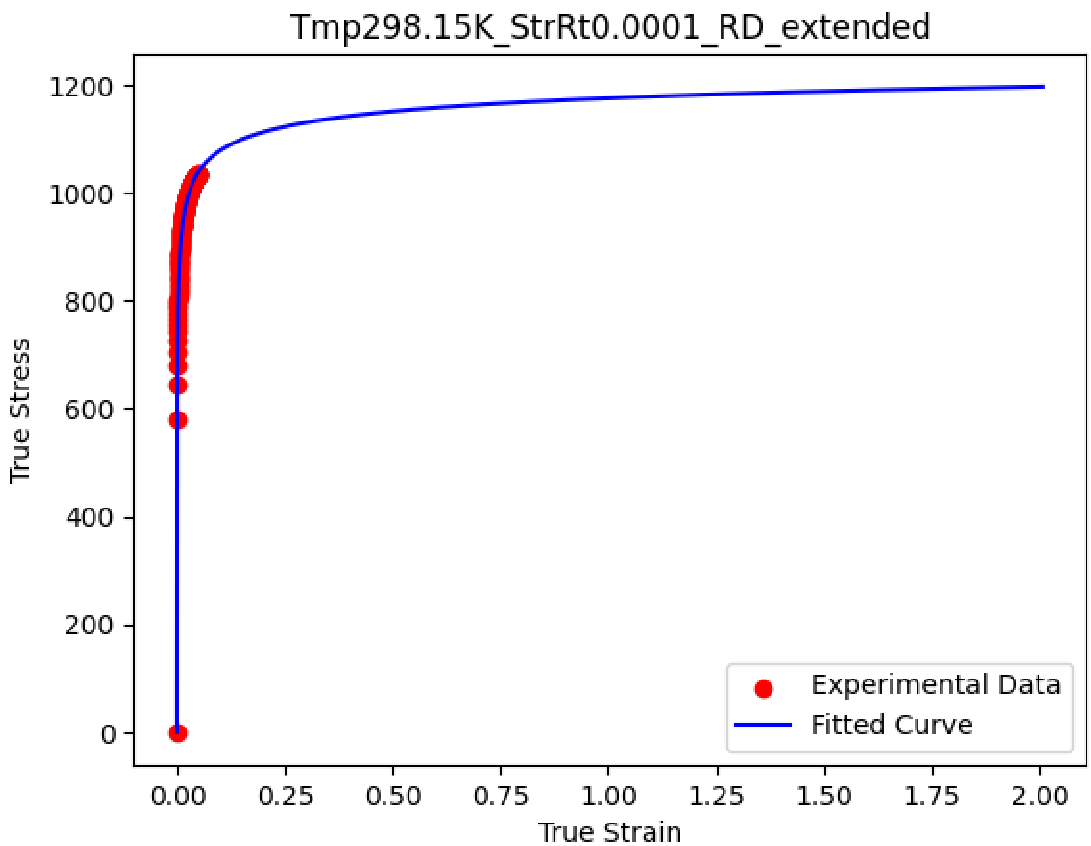
[ ]:
```
params = [] #store all parameters
params_name  = ['alpha', 'A', 'epsilon_0', 'n', 'k0', 'Q', 'beta']
```

```
conditions = ['Tmp298.15K_StrRt0.0001_RD', 'Tmp298.15K_StrRt0.0001_DD', 'Tmp298.
↪15K_StrRt0.0001_TD', 'Tmp298.15K_StrRt0.001_RD', 'Tmp298.15K_StrRt0.001_DD',␣
↪'Tmp298.15K_StrRt0.001_TD', 'Tmp298.15K_StrRt0.01_RD', 'Tmp298.15K_StrRt0.
↪01_DD', 'Tmp298.15K_StrRt0.01_TD', 'Tmp298.15K_StrRt0.1_DD', 'Tmp298.
↪15K_StrRt0.1_TD','Tmp298.15K_StrRt1_RD']
#conditions = ['Tmp77.15K_StrRt0.0001_RD']
for condition in conditions:
    params.append(analyze_sv_fit('data/Exp_FC_StrRtDpn_TmpDpn_Tmp298.csv',␣
↪condition + '_E', condition + '_S', condition))

for i in range(7):
    plt.figure(figsize=(8, 5))  # Create a new figure for each plot
    plt.plot(conditions, [p[i] for p in params], marker='o')
    plt.xlabel('Conditions')
    plt.xticks(rotation=60)
    plt.ylabel(params_name[i])
    plt.title(params_name[i] + ' of Each Condition')
    plt.tight_layout()  # Adjust layout to prevent label cut-off
    plt.show()  # Display the plot
```

```
/var/folders/n_/7tqgdxqs259f7cnfxbsjqzwm0000gp/T/ipykernel_28345/460319997.py:9:
RuntimeWarning: invalid value encountered in power
  swift_term = alpha * A * (epsilon_0 + strain) ** n
```



```
Fitted Parameters:
Alpha: -0.0843
A: 1855.4915
Epsilon_0: 0.0005
n: -0.2100
K0: 699.9021
Q: 528.6419
Beta: 12990.0817

Error Metrics:
MSE: 1.8040
RMSE: 1.3431
MAE: 1.0403
R-squared: 0.9998
```




```
/var/folders/n_/7tqgdxqs259f7cnfxbsjqzwm0000gp/T/ipykernel_28345/460319997.py:9:
RuntimeWarning: invalid value encountered in power
  swift_term = alpha * A * (epsilon_0 + strain) ** n
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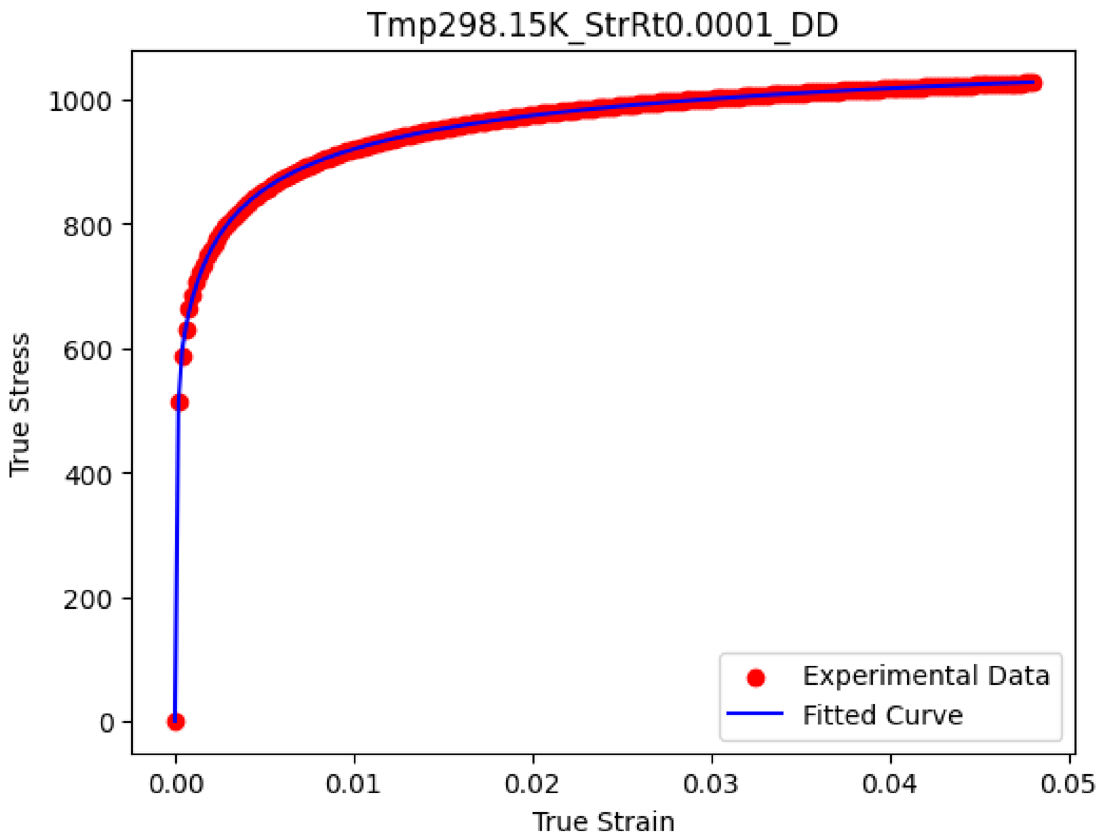
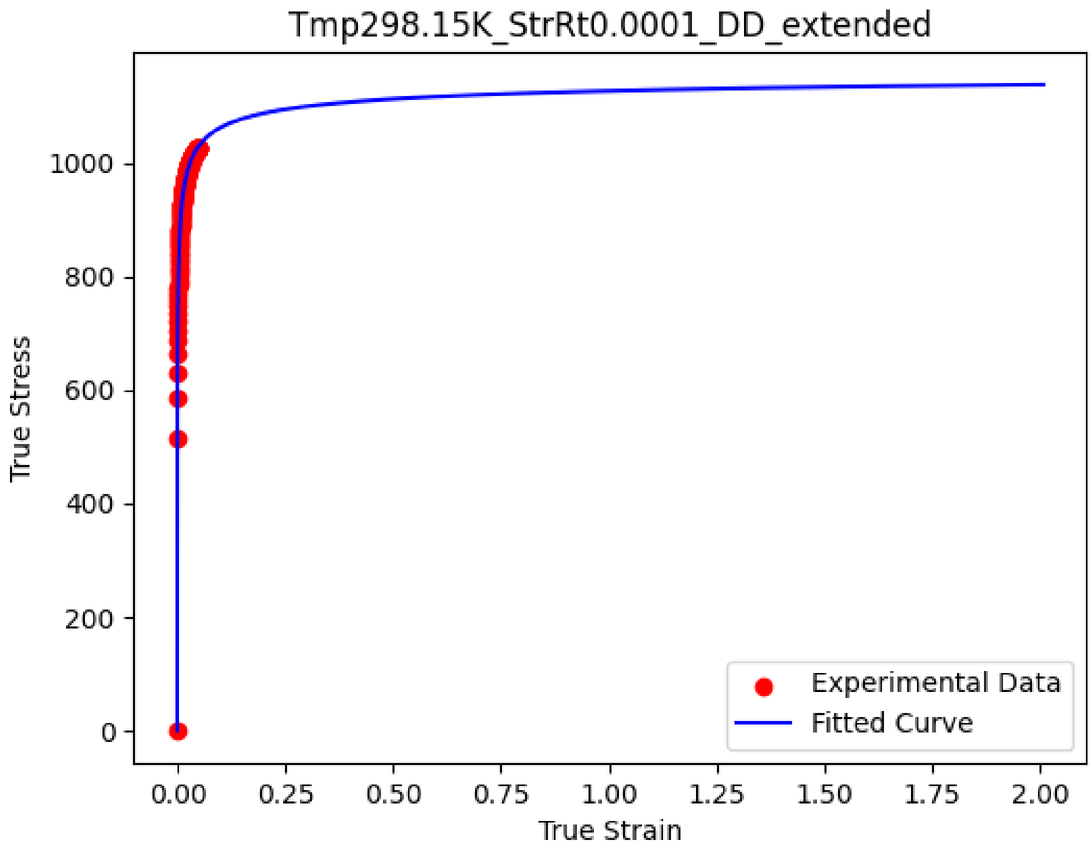
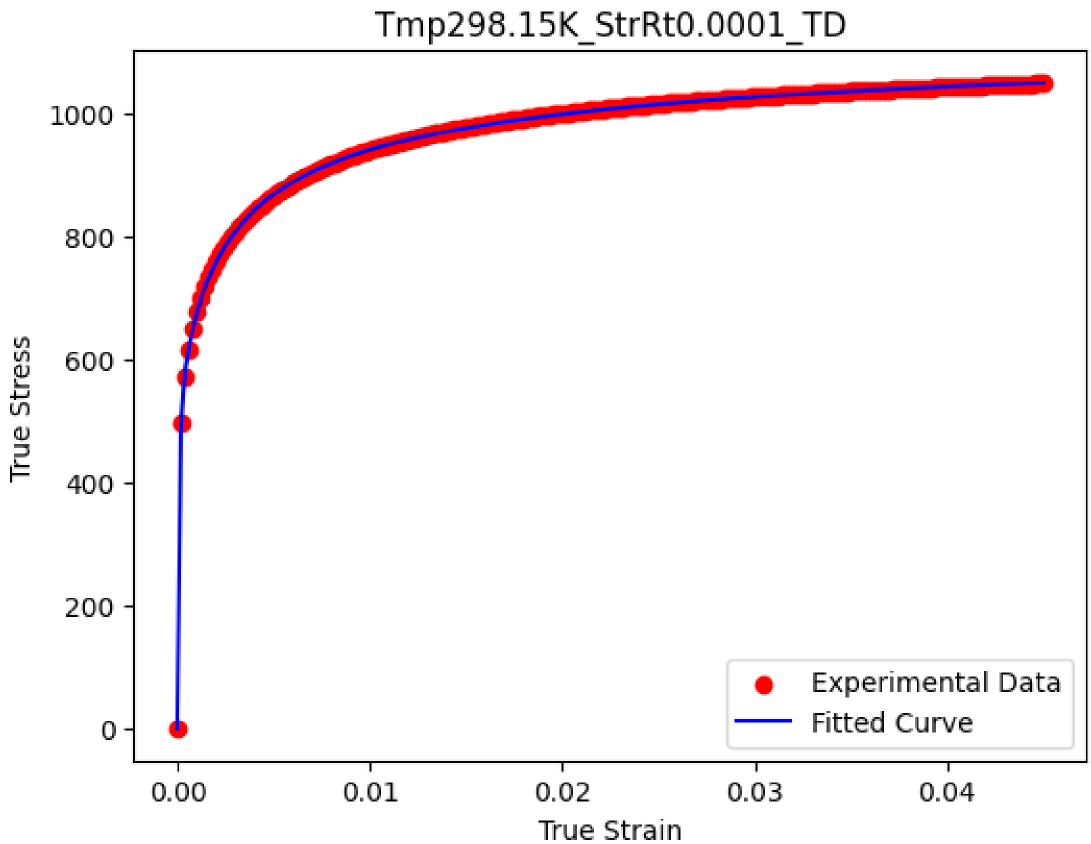


Fitted Parameters:
Alpha: -0.0351
A: 1449.0665
Epsilon_0: 0.0007
n: -0.3575
K0: 654.2613
Q: 482.9348
Beta: 11932.3490

Error Metrics:
MSE: 1.3216
RMSE: 1.1496
MAE: 0.7950
R-squared: 0.9999

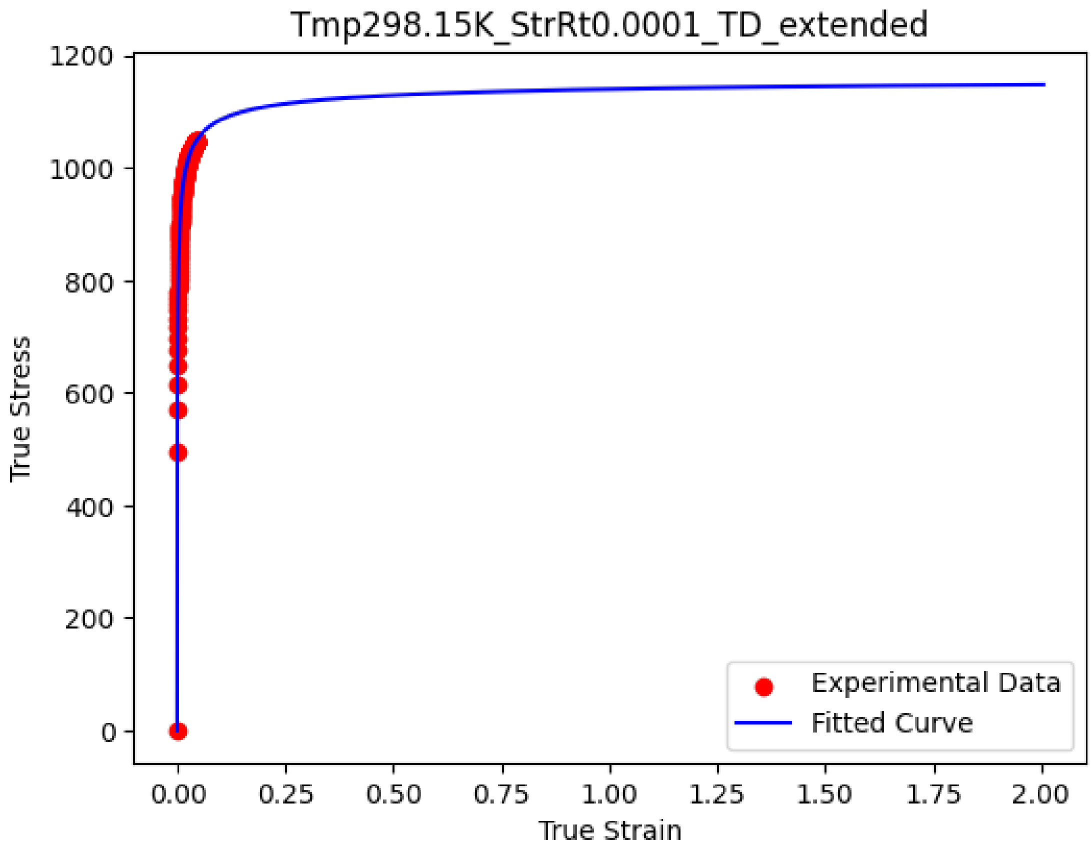



```
/var/folders/n_/7tqgdxqs259f7cnfxbsjqzwm0000gp/T/ipykernel_28345/460319997.py:9:
RuntimeWarning: invalid value encountered in power
  swift_term = alpha * A * (epsilon_0 + strain) ** n
```

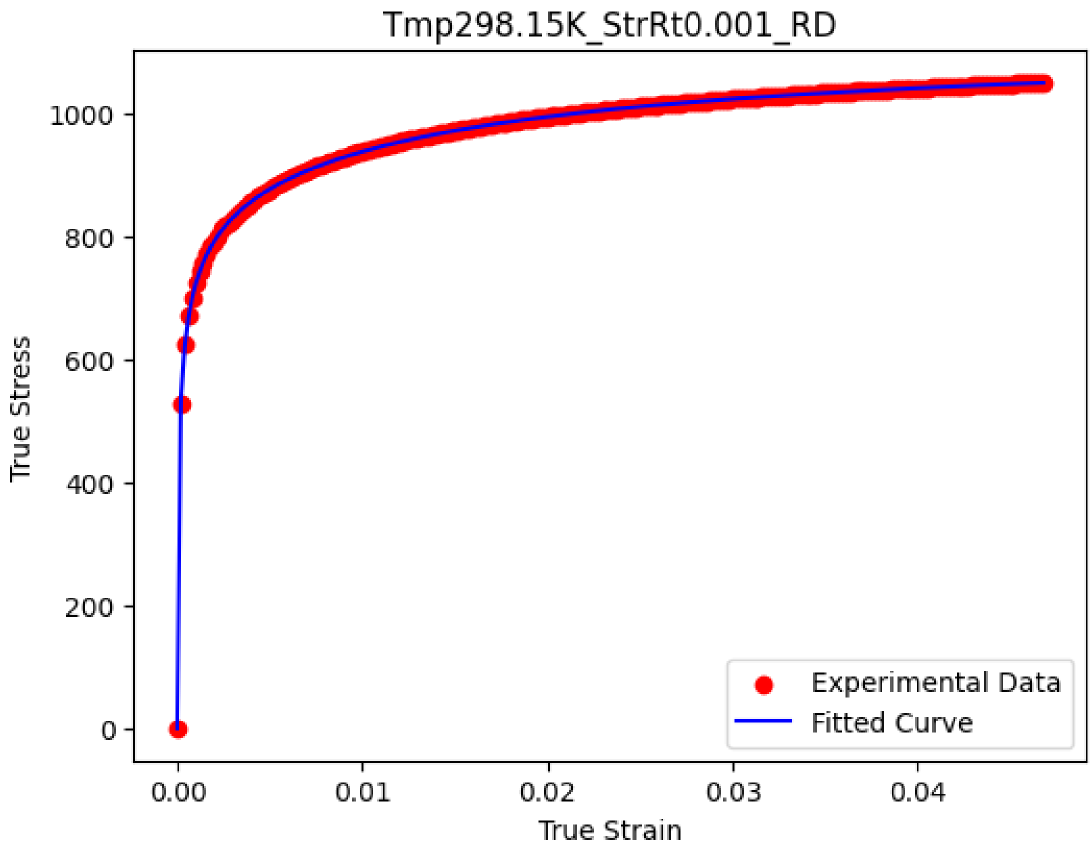



```
Fitted Parameters:
Alpha: -0.0162
A: 1859.3901
Epsilon_0: 0.0010
n: -0.4505
K0: 670.9988
Q: 480.5649
Beta: 11558.5423

Error Metrics:
MSE: 1.7418
RMSE: 1.3198
MAE: 0.9458
R-squared: 0.9999
```

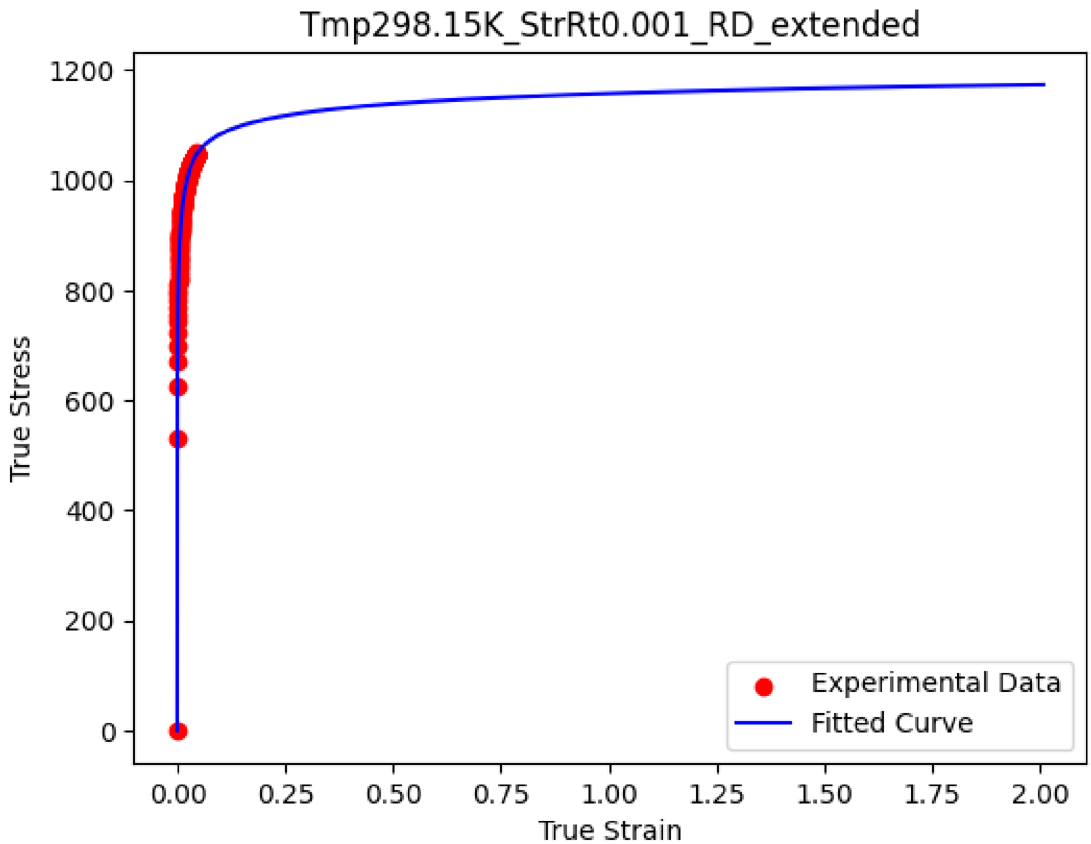



```
/var/folders/n_/7tqgdxqs259f7cnfxbsjqzwm0000gp/T/ipykernel_28345/460319997.py:9:
RuntimeWarning: invalid value encountered in power
  swift_term = alpha * A * (epsilon_0 + strain) ** n
```

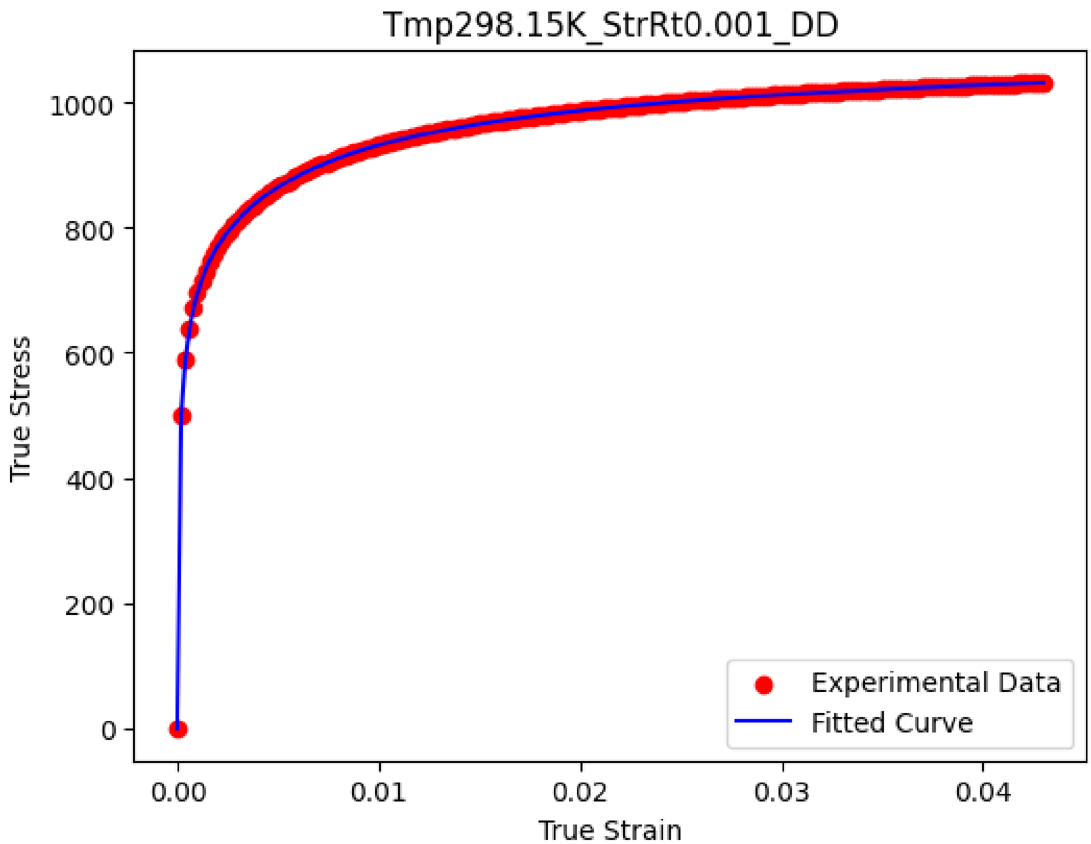



```
Fitted Parameters:
Alpha: -0.1499
A: 829.4386
Epsilon_0: 0.0000
n: -0.2021
K0: 1059.8279
Q: 54.5216
Beta: 76.6431

Error Metrics:
MSE: 0.2956
RMSE: 0.5437
MAE: 0.2610
R-squared: 1.0000
```

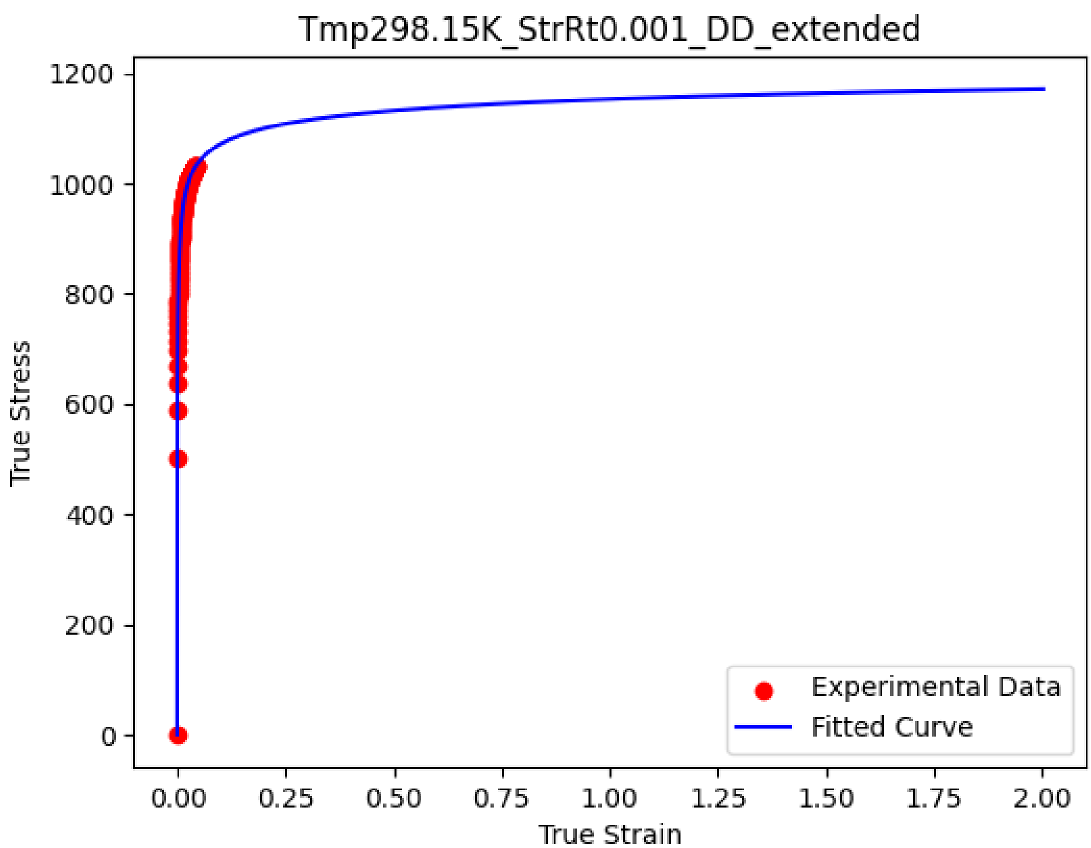



```
/var/folders/n_/7tqgdxqs259f7cnfxbsjqzwm0000gp/T/ipykernel_28345/460319997.py:9:
RuntimeWarning: invalid value encountered in power
  swift_term = alpha * A * (epsilon_0 + strain) ** n
```

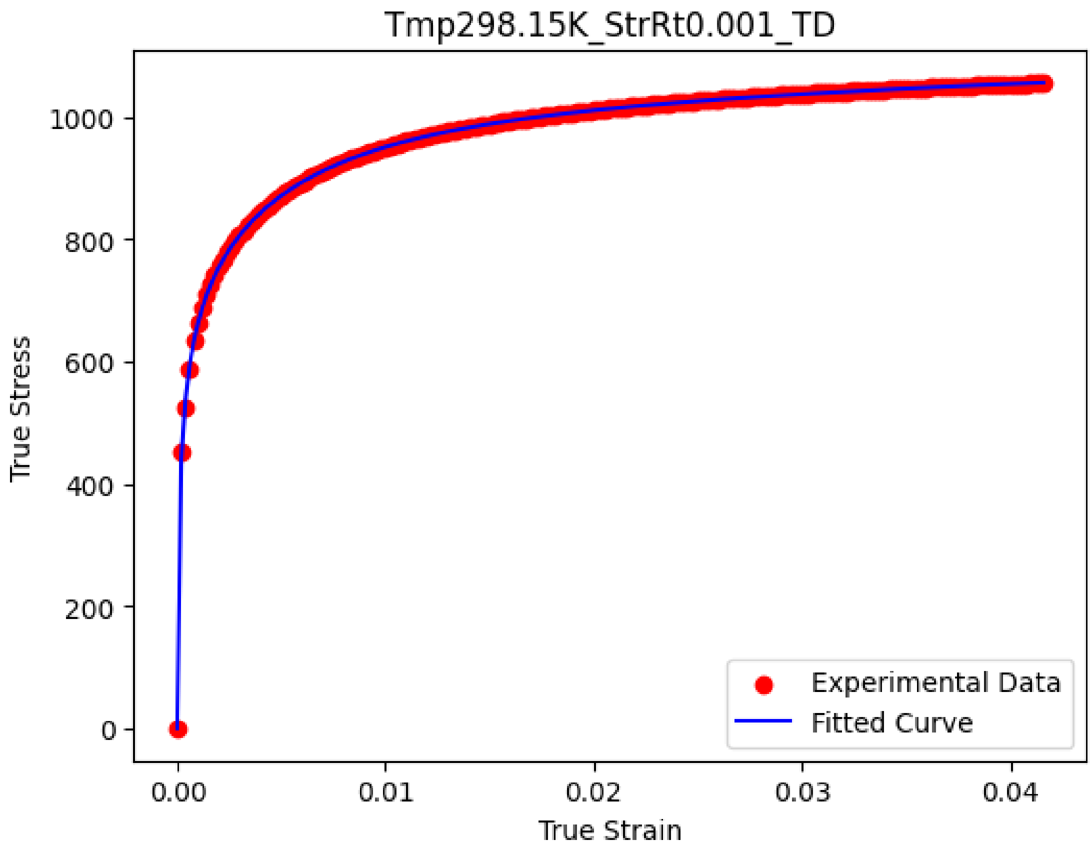



```
Fitted Parameters:
Alpha: -0.1696
A: 896.9352
Epsilon_0: 0.0000
n: -0.1862
K0: 1054.5637
Q: 61.0253
Beta: 156.4644

Error Metrics:
MSE: 0.0724
RMSE: 0.2691
MAE: 0.2127
R-squared: 1.0000
```

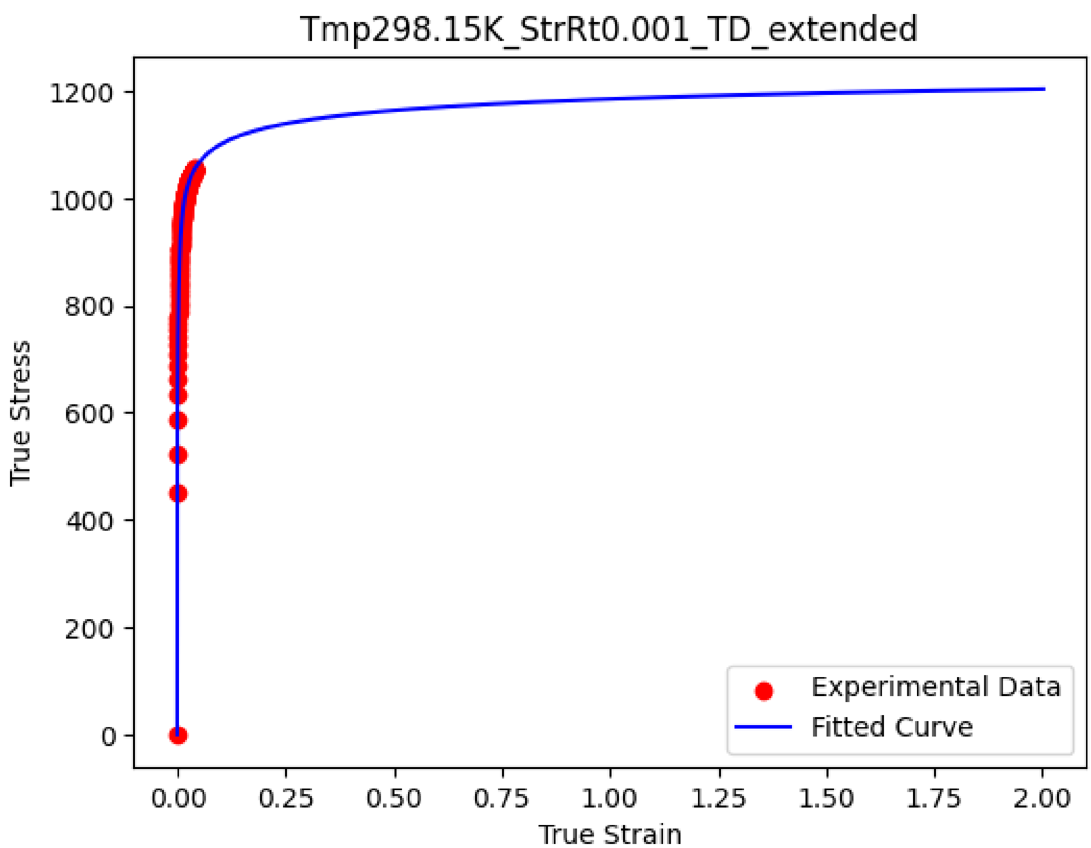



```
/var/folders/n_/7tqgdxqs259f7cnfxbsjqzwm0000gp/T/ipykernel_28345/460319997.py:9:
RuntimeWarning: invalid value encountered in power
  swift_term = alpha * A * (epsilon_0 + strain) ** n
```

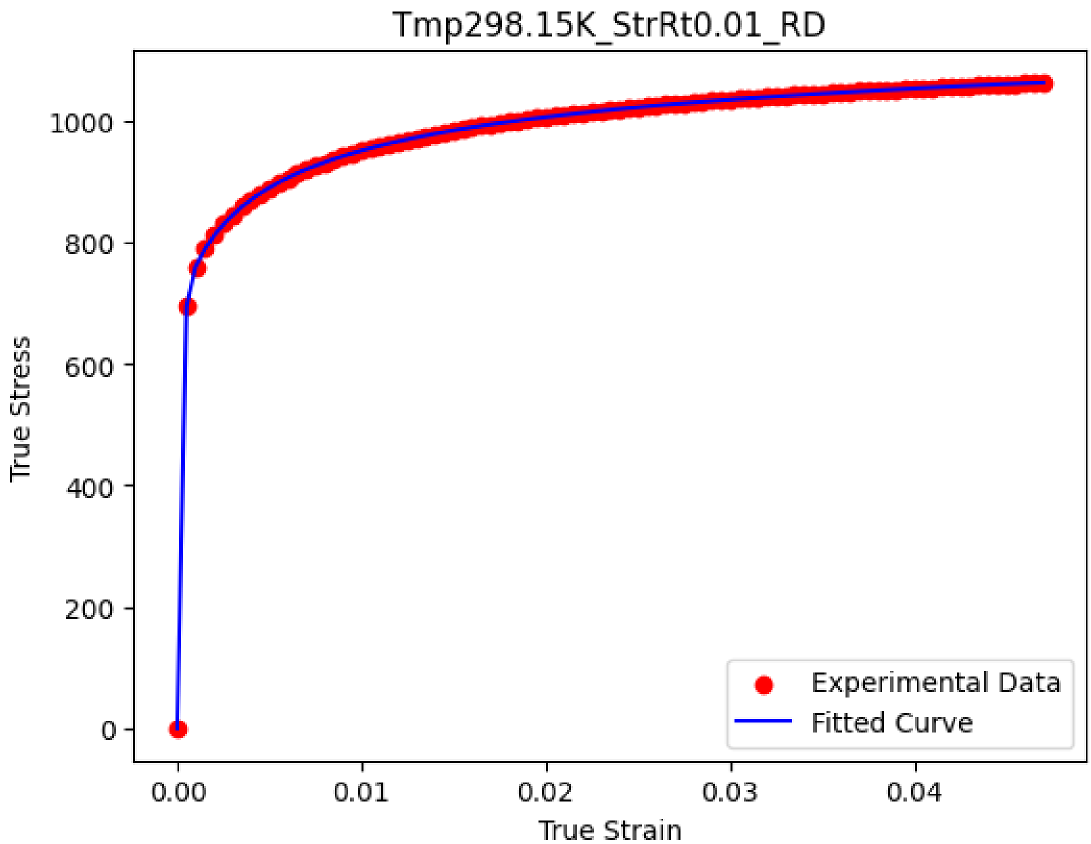



```
Fitted Parameters:
Alpha: -0.1573
A: 898.7127
Epsilon_0: 0.0000
n: -0.2040
K0: 1053.6354
Q: 92.6702
Beta: 201.5890

Error Metrics:
MSE: 2.3568
RMSE: 1.5352
MAE: 0.5065
R-squared: 0.9998
```

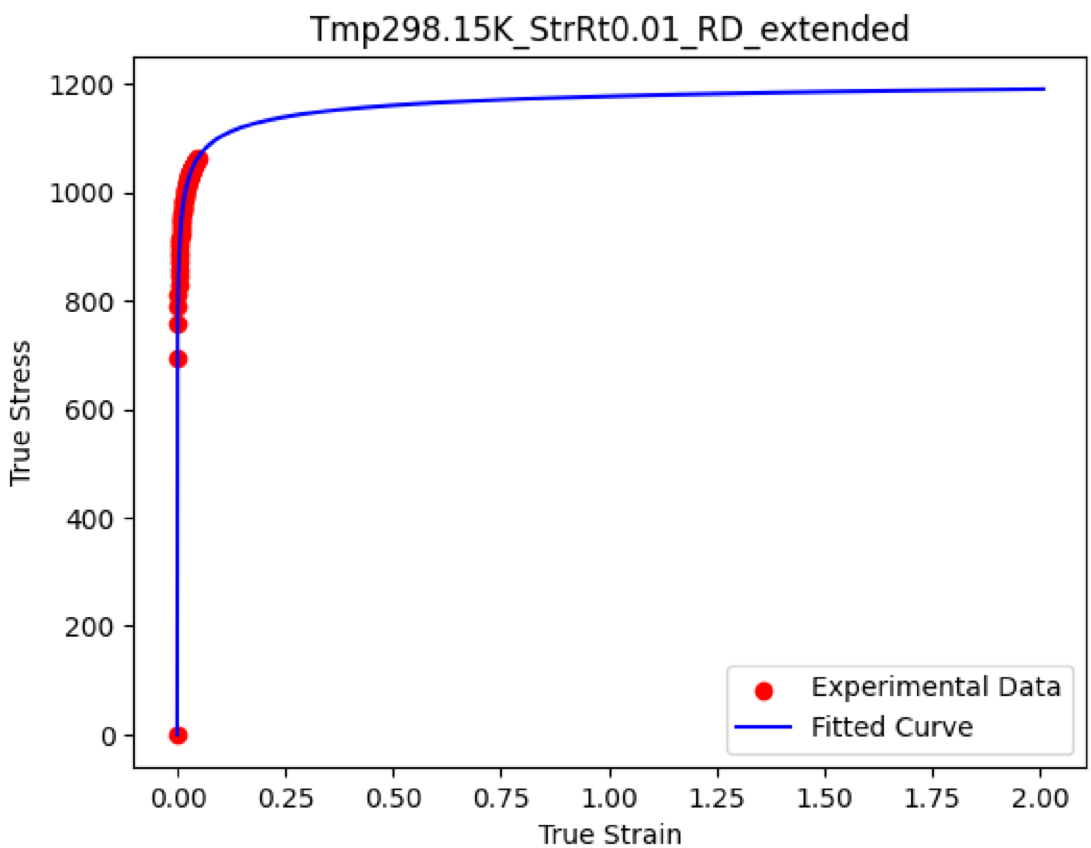



```
/var/folders/n_/7tqgdxqs259f7cnfxbsjqzwm0000gp/T/ipykernel_28345/460319997.py:9:
RuntimeWarning: invalid value encountered in power
  swift_term = alpha * A * (epsilon_0 + strain) ** n
```



Fitted Parameters:
Alpha: -0.0412
A: 1528.7965
Epsilon_0: 0.0017
n: -0.3426
K0: 538.6508
Q: 652.1925
Beta: 6113.3657

Error Metrics:
MSE: 0.2257
RMSE: 0.4751
MAE: 0.3518
R-squared: 1.0000

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/var/folders/n_/7tqgdxqs259f7cnfxbsjqzwm0000gp/T/ipykernel_28345/460319997.py:9:
RuntimeWarning: invalid value encountered in power
  swift_term = alpha * A * (epsilon_0 + strain) ** n
```
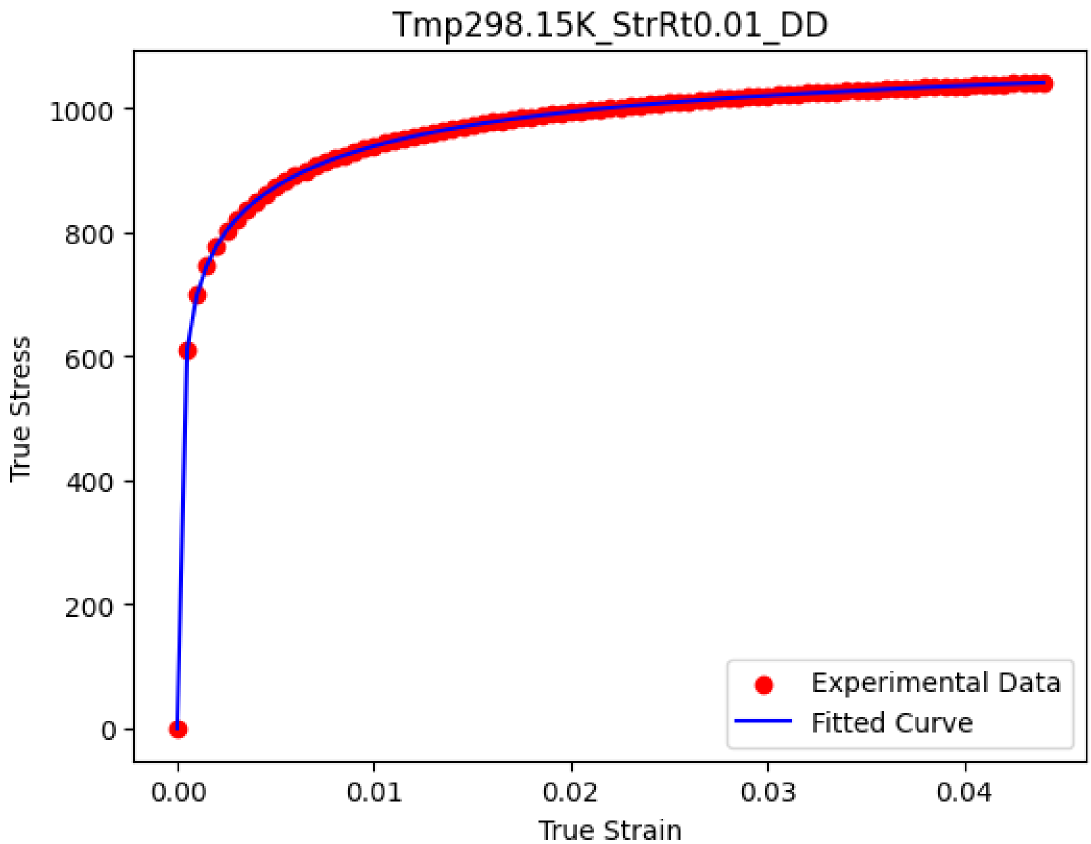
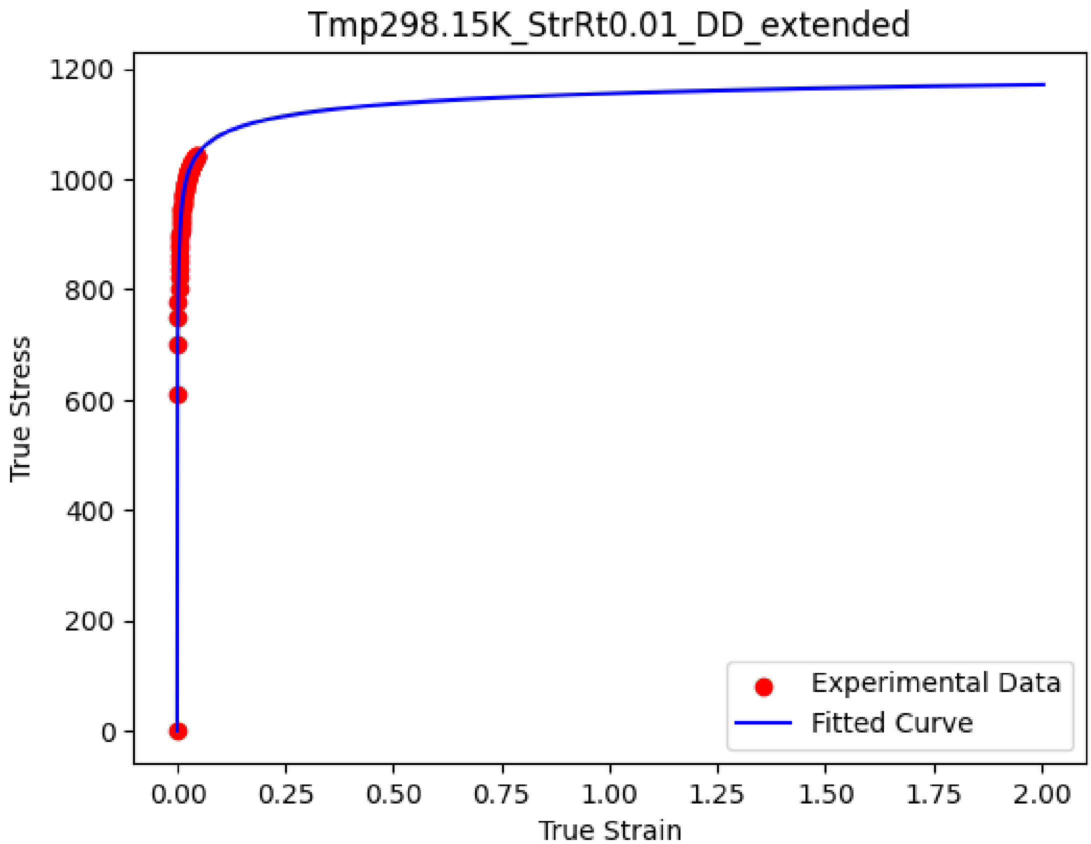
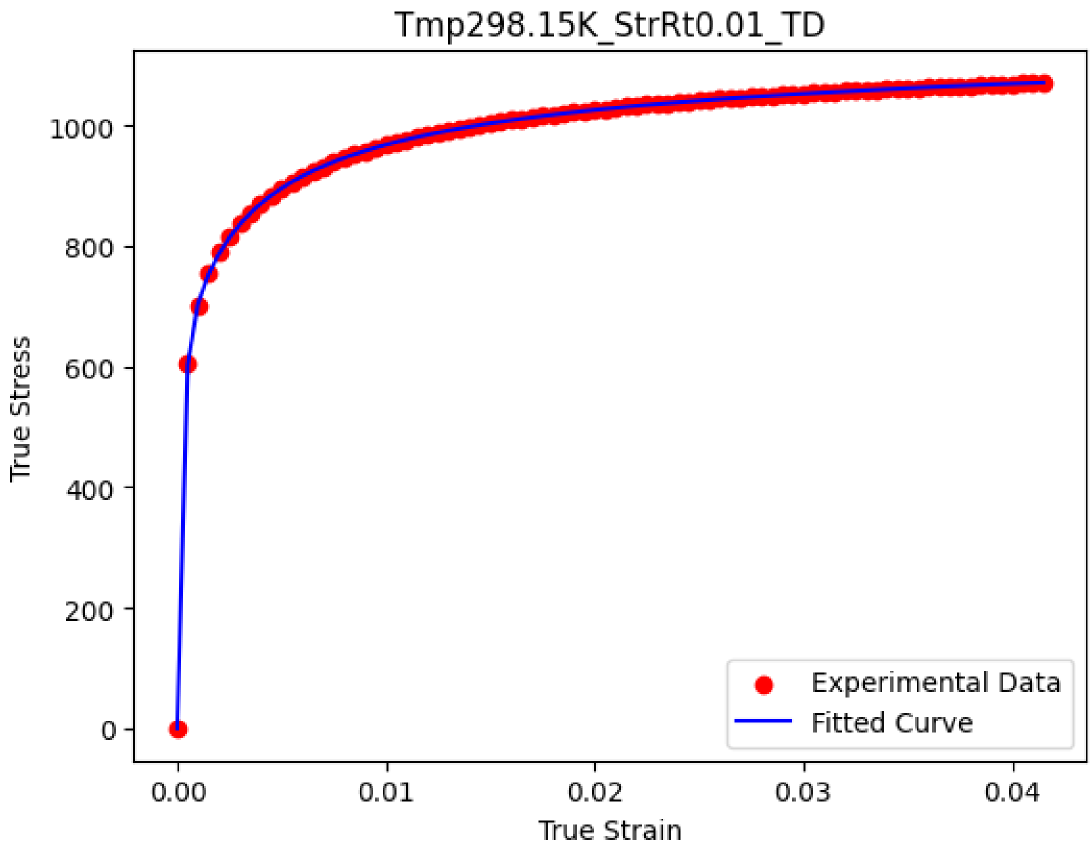



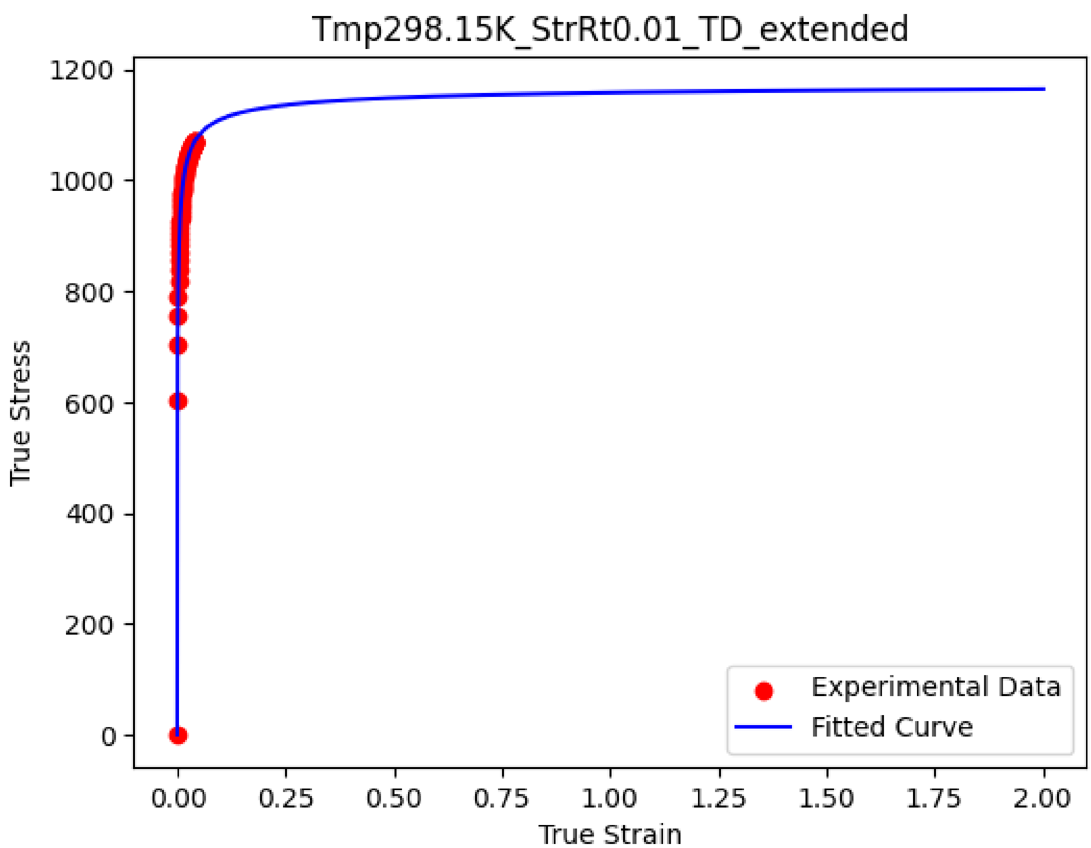

```
Fitted Parameters:
Alpha: -0.1439
A: 786.6893
Epsilon_0: 0.0000
n: -0.2221
K0: 1062.3852
Q: 46.3042
Beta: 130.3721

Error Metrics:
MSE: 0.2331
RMSE: 0.4828
MAE: 0.2647
R-squared: 1.0000
```



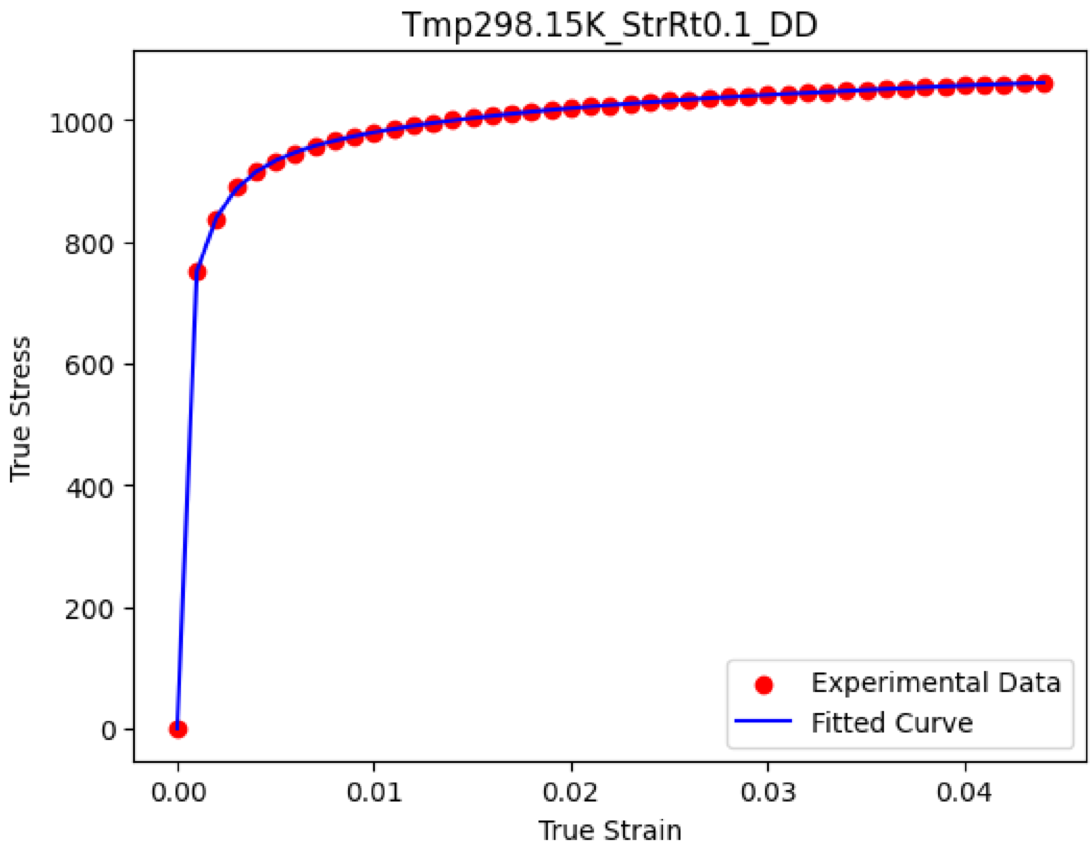

```
/var/folders/n_/7tqgdxqs259f7cnfxbsjqzwm0000gp/T/ipykernel_28345/460319997.py:9:
RuntimeWarning: invalid value encountered in power
  swift_term = alpha * A * (epsilon_0 + strain) ** n
```



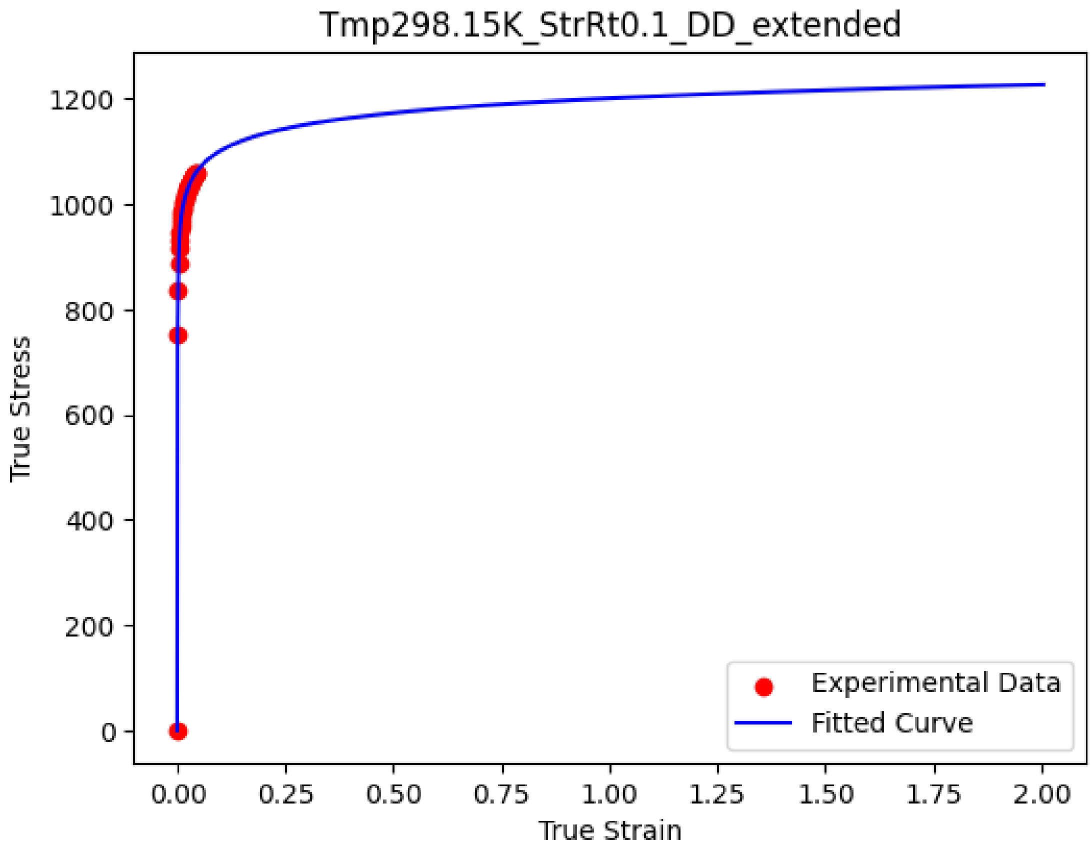

```
Fitted Parameters:
Alpha: -0.0142
A: 1595.8106
Epsilon_0: 0.0013
n: -0.4994
K0: 620.4402
Q: 543.5982
Beta: 5095.2831

Error Metrics:
MSE: 0.4123
RMSE: 0.6421
MAE: 0.4282
R-squared: 1.0000
```



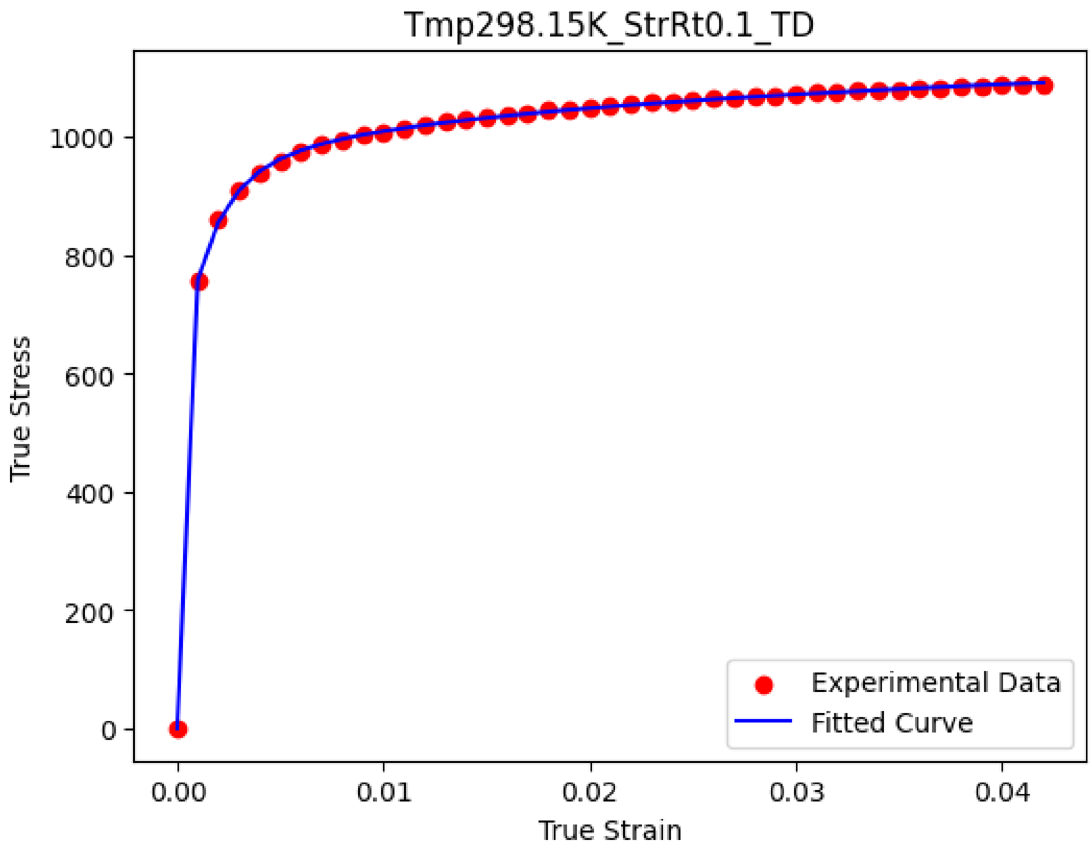

```
/var/folders/n_/7tqgdxqs259f7cnfxbsjqzwm0000gp/T/ipykernel_28345/460319997.py:9:
RuntimeWarning: invalid value encountered in power
  swift_term = alpha * A * (epsilon_0 + strain) ** n
```



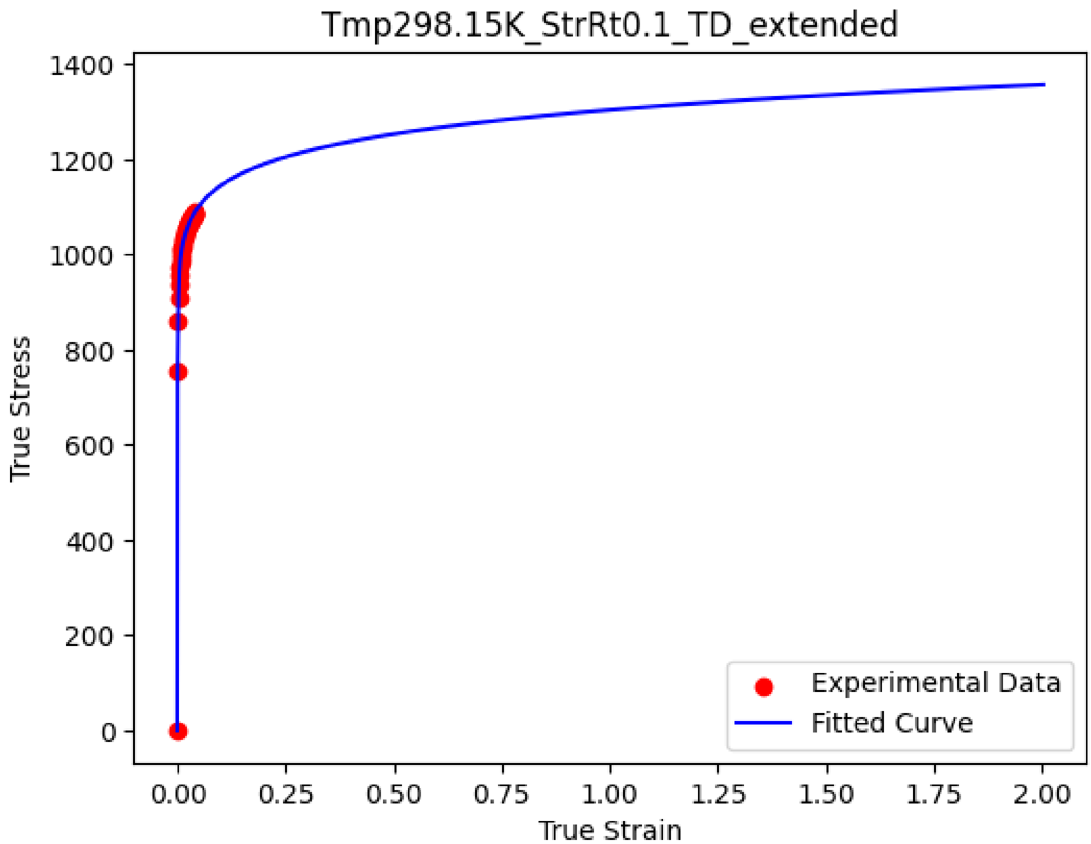

```
Fitted Parameters:
Alpha: -0.2393
A: 1821.1632
Epsilon_0: 0.0000
n: -0.0894
K0: 1192.5889
Q: 128.4945
Beta: 718.7260

Error Metrics:
MSE: 0.6722
RMSE: 0.8199
MAE: 0.3893
R-squared: 1.0000
```



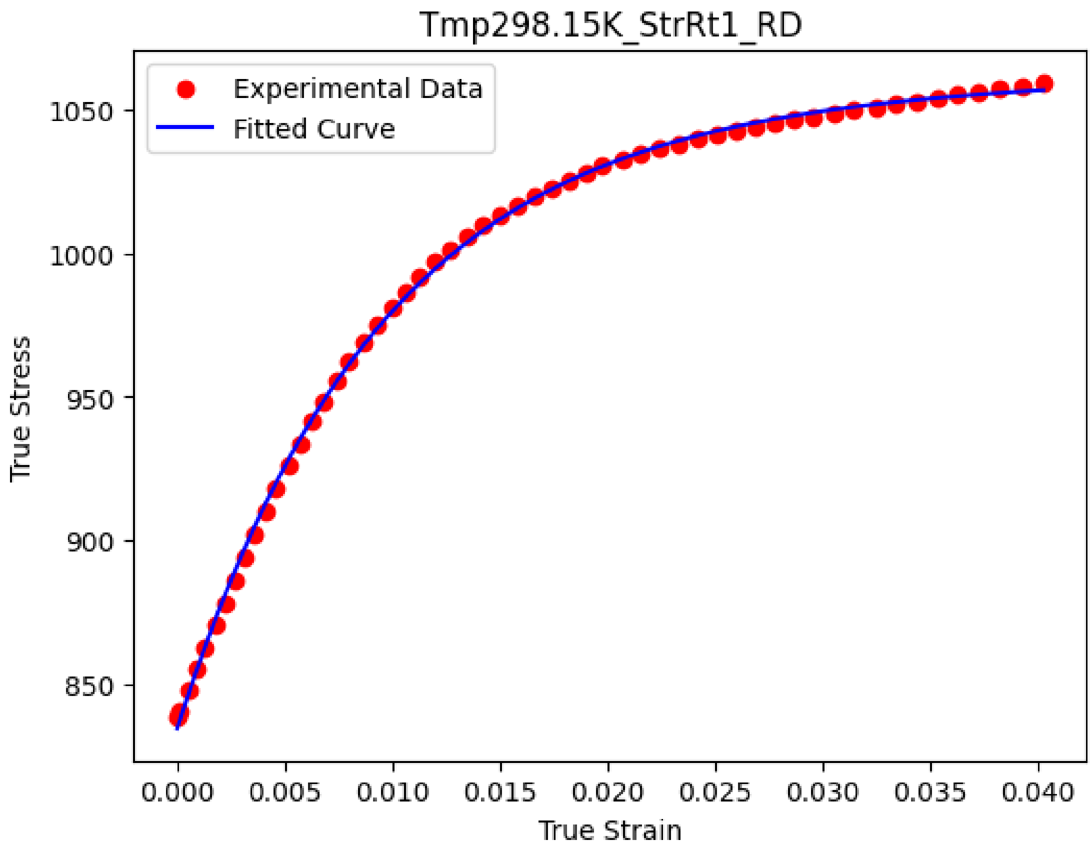

```
/var/folders/n_/7tqgdxqs259f7cnfxbsjqzwm0000gp/T/ipykernel_28345/460319997.py:9:
RuntimeWarning: invalid value encountered in power
  swift_term = alpha * A * (epsilon_0 + strain) ** n
```



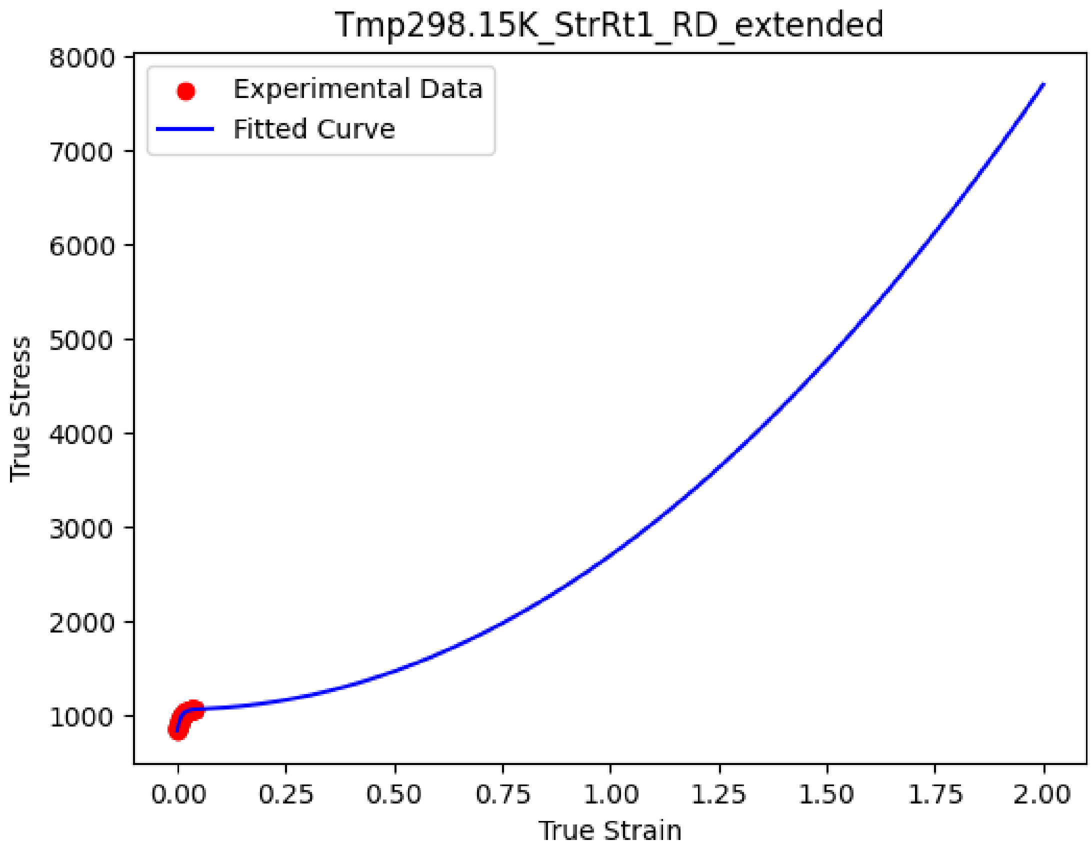

```
Fitted Parameters:
Alpha: 0.8197
A: 1290.7194
Epsilon_0: 0.0000
n: 0.0709
K0: -60.3743
Q: 1426.2732
Beta: 638.7484

Error Metrics:
MSE: 3.2585
RMSE: 1.8051
MAE: 1.4837
R-squared: 0.9999
```



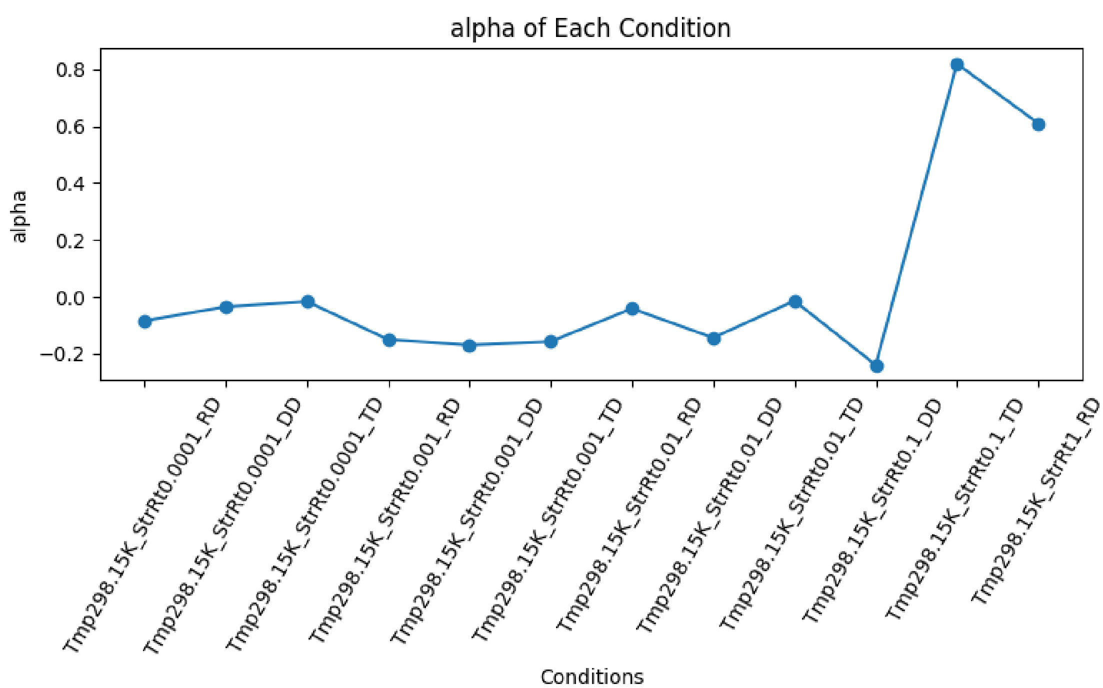

```
/var/folders/n_/7tqgdxqs259f7cnfxbsjqzwm0000gp/T/ipykernel_28345/460319997.py:9:
RuntimeWarning: invalid value encountered in power
  swift_term = alpha * A * (epsilon_0 + strain) ** n
```



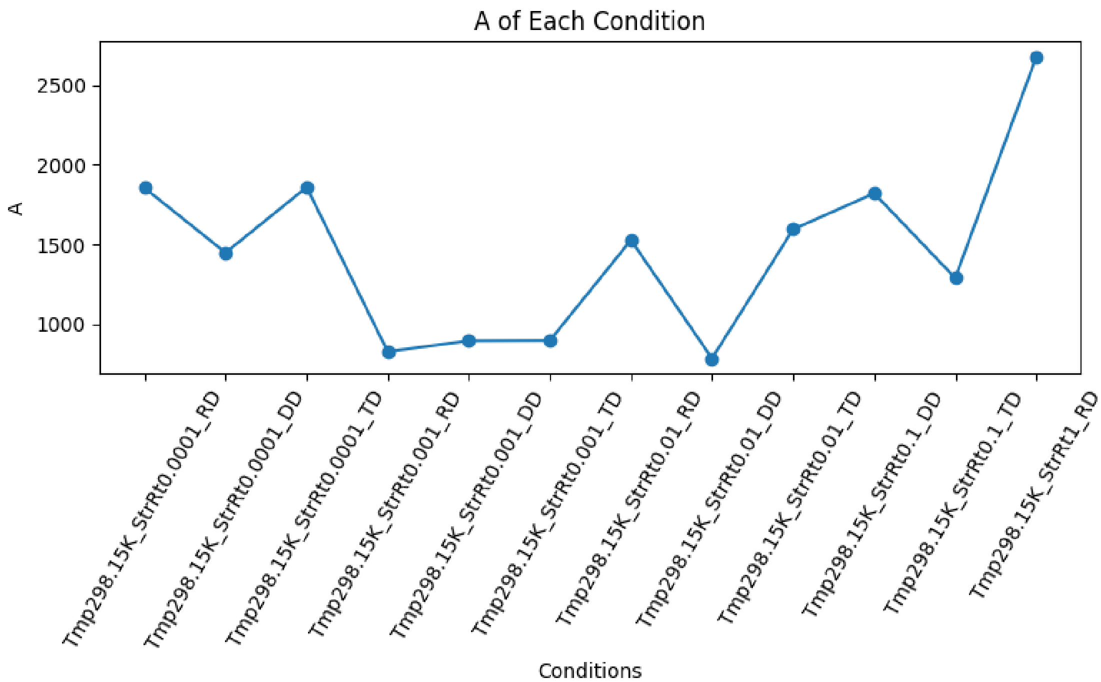

```
Fitted Parameters:
Alpha: 0.6101
A: 2676.8427
Epsilon_0: 0.0000
n: 2.0233
K0: 2140.0914
Q: 572.5317
Beta: 105.0464

Error Metrics:
MSE: 2.8767
RMSE: 1.6961
MAE: 1.4310
R-squared: 0.9994
```

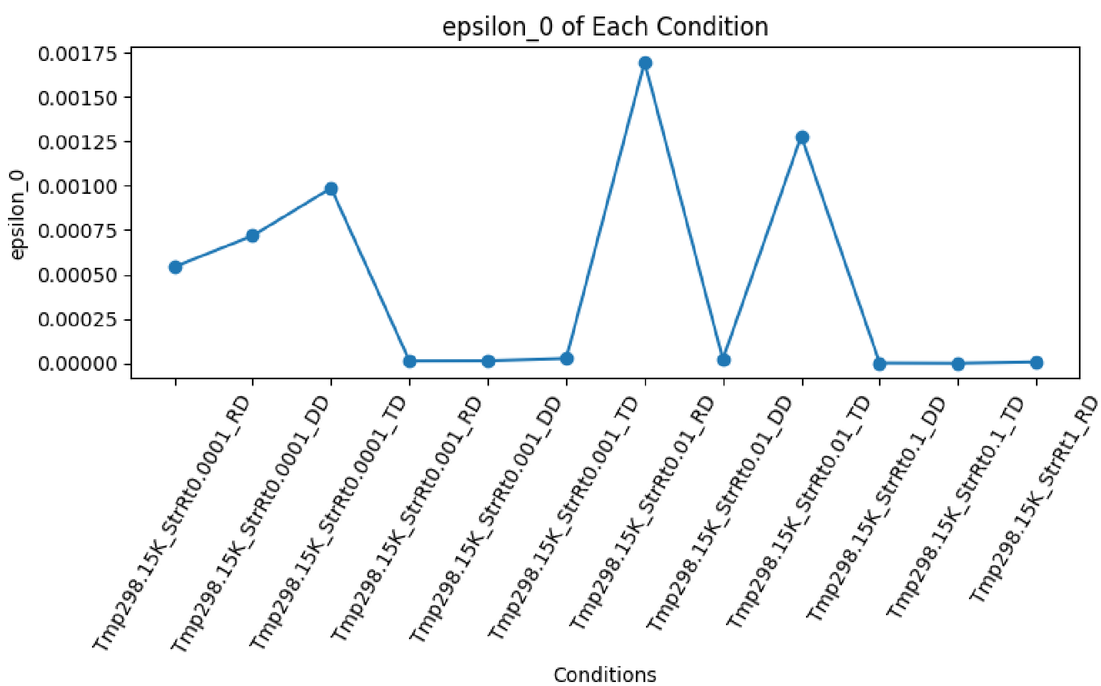


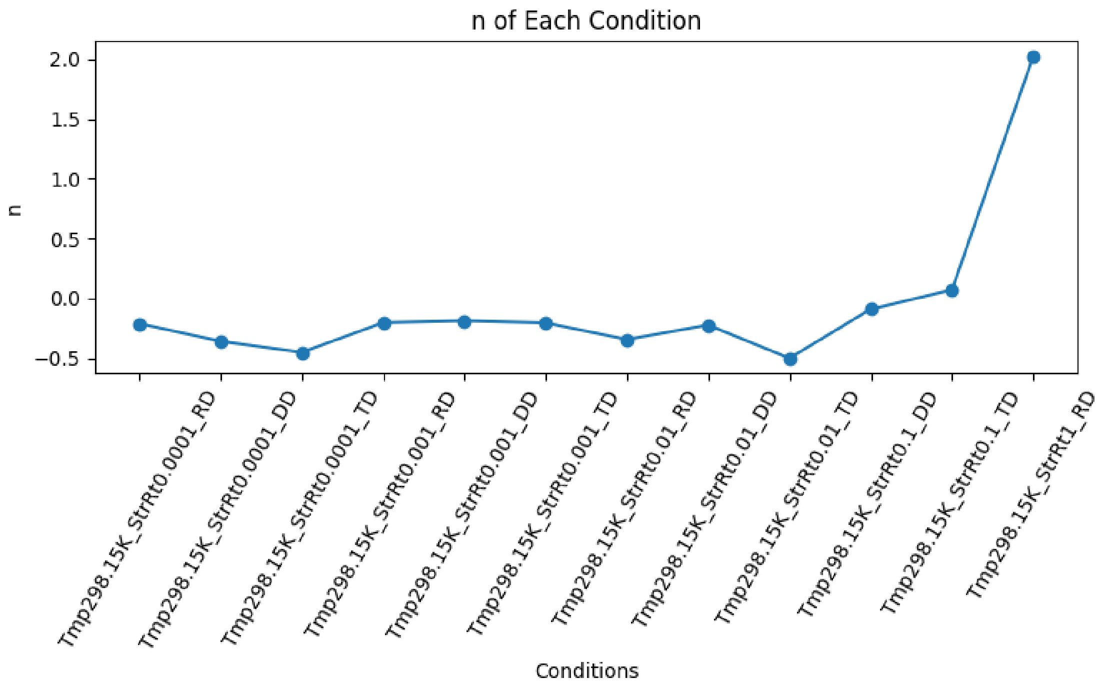
Tmp298.15K_StrRt1_RD_extended
Experimental Data
Fitted Curve
True Stress
True Strain
8000
7000
6000
5000
4000
3000
2000
1000
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00

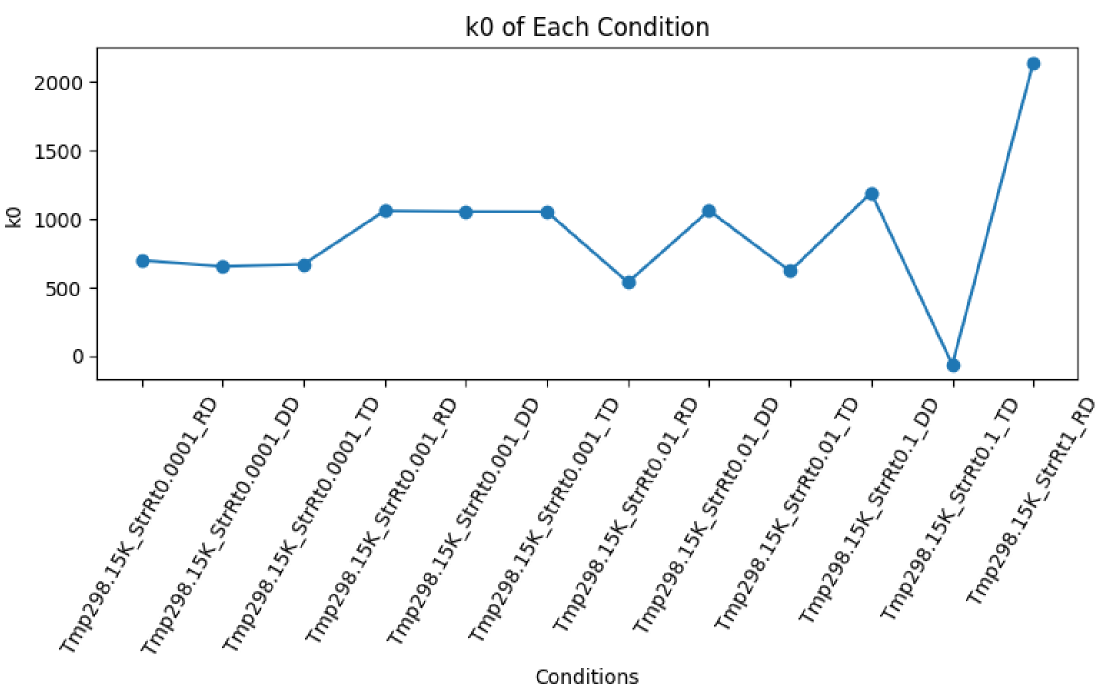


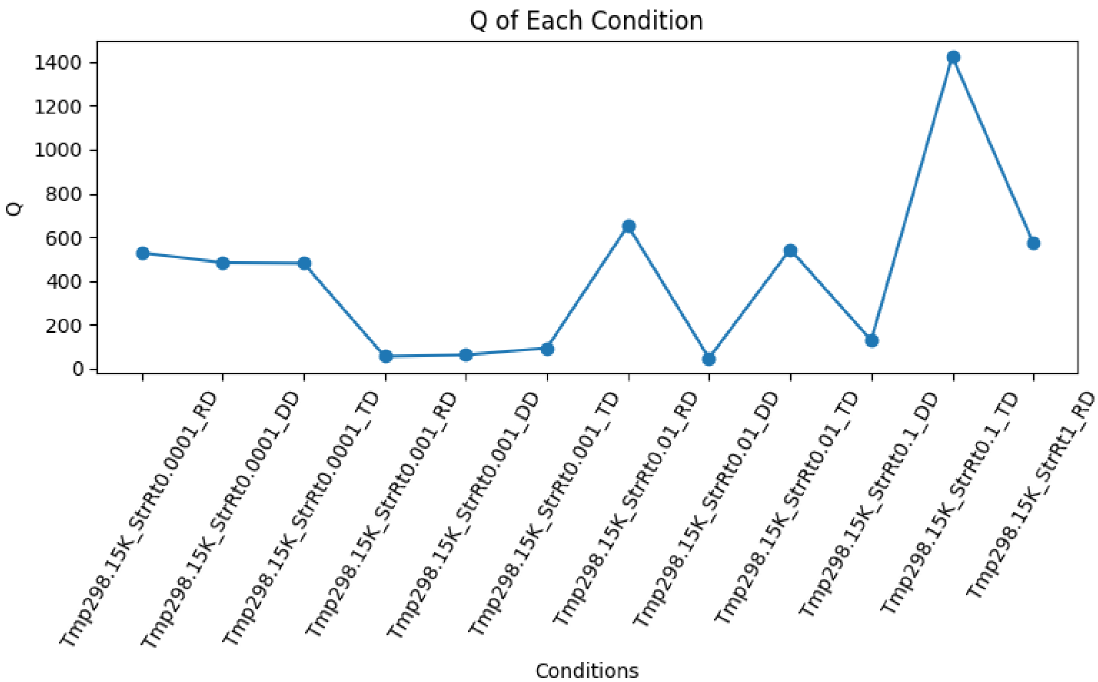
alpha of Each Condition
alpha
Conditions
0.8
0.6
0.4
0.2
0.0
−0.2
Tmp298.15K_StrRt0.0001_RD
Tmp298.15K_StrRt0.0001_DD
Tmp298.15K_StrRt0.0001_TD
Tmp298.15K_StrRt0.001_RD
Tmp298.15K_StrRt0.001_DD
Tmp298.15K_StrRt0.001_TD
Tmp298.15K_StrRt0.01_RD
Tmp298.15K_StrRt0.01_DD
Tmp298.15K_StrRt0.01_TD
Tmp298.15K_StrRt0.1_DD
Tmp298.15K_StrRt0.1_TD
Tmp298.15K_StrRt1_RD

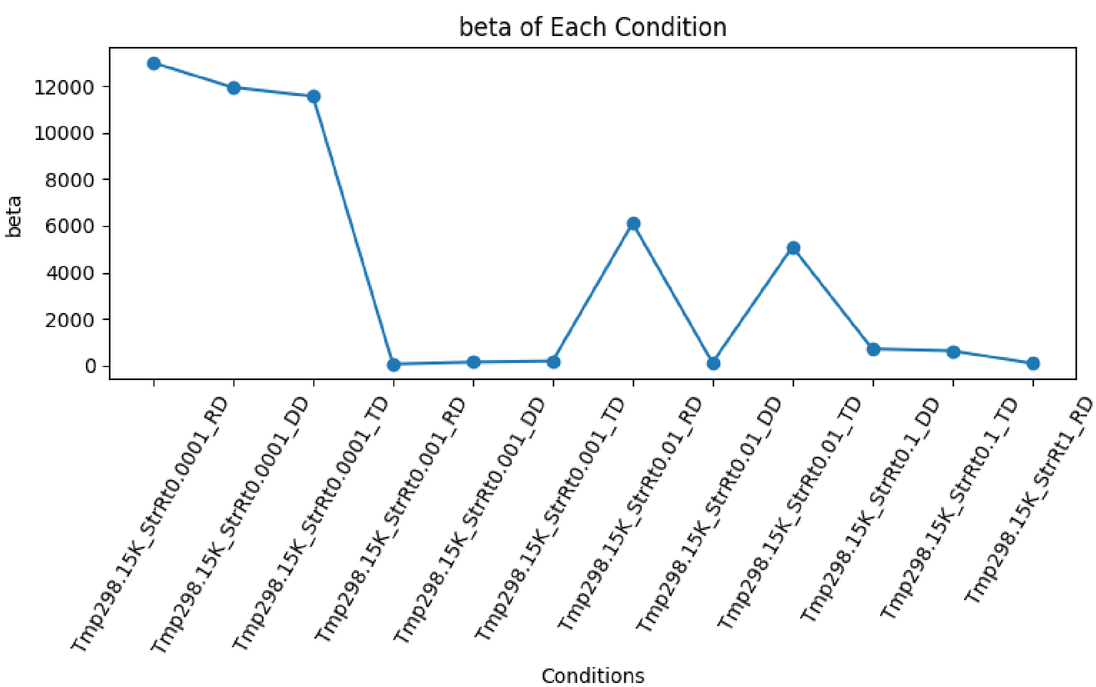

A of Each Condition
A
2500
2000
1500
1000
Tmp298.15K_StrRt0.0001_RD
Tmp298.15K_StrRt0.0001_DD
Tmp298.15K_StrRt0.0001_TD
Tmp298.15K_StrRt0.001_RD
Tmp298.15K_StrRt0.001_DD
Tmp298.15K_StrRt0.001_TD
Tmp298.15K_StrRt0.01_RD
Tmp298.15K_StrRt0.01_DD
Tmp298.15K_StrRt0.01_TD
Tmp298.15K_StrRt0.1_DD
Tmp298.15K_StrRt0.1_TD
Tmp298.15K_StrRt1_RD
Conditions


epsilon_0 of Each Condition
epsilon_0
0.00175
0.00150
0.00125
0.00100
0.00075
0.00050
0.00025
0.00000
Tmp298.15K_StrRt0.0001_RD
Tmp298.15K_StrRt0.0001_DD
Tmp298.15K_StrRt0.0001_TD
Tmp298.15K_StrRt0.001_RD
Tmp298.15K_StrRt0.001_DD
Tmp298.15K_StrRt0.001_TD
Tmp298.15K_StrRt0.01_RD
Tmp298.15K_StrRt0.01_DD
Tmp298.15K_StrRt0.01_TD
Tmp298.15K_StrRt0.1_DD
Tmp298.15K_StrRt0.1_TD
Tmp298.15K_StrRt1_RD
Conditions


n of Each Condition
2.0
1.5
1.0
0.5
0.0
−0.5
n
Tmp298.15K_StrRt0.0001_RD
Tmp298.15K_StrRt0.0001_DD
Tmp298.15K_StrRt0.0001_TD
Tmp298.15K_StrRt0.001_RD
Tmp298.15K_StrRt0.001_DD
Tmp298.15K_StrRt0.001_TD
Tmp298.15K_StrRt0.01_RD
Tmp298.15K_StrRt0.01_DD
Tmp298.15K_StrRt0.01_TD
Tmp298.15K_StrRt0.1_DD
Tmp298.15K_StrRt0.1_TD
Tmp298.15K_StrRt1_RD
Conditions


k0 of Each Condition
2000
1500
1000
500
0
k0
Tmp298.15K_StrRt0.0001_RD
Tmp298.15K_StrRt0.0001_DD
Tmp298.15K_StrRt0.0001_TD
Tmp298.15K_StrRt0.001_RD
Tmp298.15K_StrRt0.001_DD
Tmp298.15K_StrRt0.001_TD
Tmp298.15K_StrRt0.01_RD
Tmp298.15K_StrRt0.01_DD
Tmp298.15K_StrRt0.01_TD
Tmp298.15K_StrRt0.1_DD
Tmp298.15K_StrRt0.1_TD
Tmp298.15K_StrRt1_RD
Conditions


Q of Each Condition
Q
1400
1200
1000
800
600
400
200
0
Tmp298.15K_StrRt0.0001_RD
Tmp298.15K_StrRt0.0001_DD
Tmp298.15K_StrRt0.0001_TD
Tmp298.15K_StrRt0.001_RD
Tmp298.15K_StrRt0.001_DD
Tmp298.15K_StrRt0.001_TD
Tmp298.15K_StrRt0.01_RD
Tmp298.15K_StrRt0.01_DD
Tmp298.15K_StrRt0.01_TD
Tmp298.15K_StrRt0.1_DD
Tmp298.15K_StrRt0.1_TD
Tmp298.15K_StrRt1_RD
Conditions


beta of Each Condition
beta
12000
10000
8000
6000
4000
2000
0
Tmp298.15K_StrRt0.0001_RD
Tmp298.15K_StrRt0.0001_DD
Tmp298.15K_StrRt0.0001_TD
Tmp298.15K_StrRt0.001_RD
Tmp298.15K_StrRt0.001_DD
Tmp298.15K_StrRt0.001_TD
Tmp298.15K_StrRt0.01_RD
Tmp298.15K_StrRt0.01_DD
Tmp298.15K_StrRt0.01_TD
Tmp298.15K_StrRt0.1_DD
Tmp298.15K_StrRt0.1_TD
Tmp298.15K_StrRt1_RD
Conditions