Transverse CPGE

Low-Frequency Peak

Group of: Prof. Guoqing Chang

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Original POSCAR

```
Primitive Cell
 1.000000
   7.4800        0        0
        0   8.6160   -2.8040
        0   8.6160    2.8040
 S  Ta
 8  12
 direct
  0.8270000000  0.8476000000  0.0728000000
  0.1730000000  0.9272000000  0.1524000000
  0.8270000000  0.4272000000  0.6524000000
  0.1730000000  0.3476000000  0.5728000000
  0.5843000000  0.2692000000  0.5000000000
  0.4157000000  0.5000000000  0.7308000000
  0.5843000000  0.0000000000  0.2308000000
  0.4157000000  0.7692000000  0.0000000000
  0.7189600000  0.5895100000  0.0781100000
  0.2810400000  0.9218900000  0.4104900000
  0.7189600000  0.4218900000  0.9104900000
  0.2810400000  0.0895100000  0.5781100000
  0.1045500000  0.6546000000  0.1308000000
  0.8954500000  0.8692000000  0.3454000000
  0.1045500000  0.3692000000  0.8454000000
  0.8954500000  0.1546000000  0.6308000000
  0.6551000000  0.0263000000  0.4737000000
  0.3449000000  0.5263000000  0.9737000000
  0.9942000000  0.7609000000  0.7391000000
  0.0058000000  0.2609000000  0.2391000000
```

From the provided POSCAR data, the lattice vectors are given by:

$$\boldsymbol{a} = \begin{bmatrix} 7.4800 \\ 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} 0 \\ 8.6160 \\ -2.8040 \end{bmatrix}, \quad \boldsymbol{c} = \begin{bmatrix} 0 \\ 8.6160 \\ 2.8040 \end{bmatrix}$$

Where $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$ are the lattice vectors of the unit cell.

The lengths of the lattice vectors are:

$$|\,\boldsymbol{a}\,| = 7.4800\ A^{\circ}$$
$$|\,\boldsymbol{b}\,| = 9.0608\ A^{\circ}$$
$$|\,\boldsymbol{c}\,| = 9.0608\ A^{\circ}$$

So, the values for $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$ in the unit cell are 7.4800 Å, 9.0608 Å, and 9.0608 Å respectively.

Effects of tilted velocity

$$\mathcal{H}(\mathbf{k}) = \sum_{i=x,y,z} (\nu_i^t \hbar k_i + \nu_i \hbar k_i \sigma_i) - \mu$$

The CPGE tensor for the tilted term in the Weyl Hamiltonian as follows

$$\beta_{ij} = \frac{3e^3 \,\mathrm{sgn}(\mathcal{C})}{\pi h^2} \left[\frac{\nu_i^t \nu_j^t}{\nu_j^2} \frac{1}{\mathcal{W_T}^2} \sum_{n=1}^{2} (-1)^n \sin(\gamma_n) \cos(\gamma_n)^3 \right]$$

with

$$\gamma_n = \arcsin\{\frac{1}{\mathcal{W_T}}[\frac{2|\mu|}{\hbar\omega} + (-1)^{n+1}]\}$$

$$\mathcal{W_T} = \sqrt{(\frac{\nu_x^t}{\nu_x})^2 + (\frac{\nu_y^t}{\nu_y})^2 + (\frac{\nu_z^t}{\nu_z})^2}$$

Model

The maximum value of β_{ij} is profoundly affected by

$$\begin{cases} \dfrac{\nu_i^t}{\nu_i} = \dfrac{\nu_j^t}{\nu_j} \\ \dfrac{\nu_k^t}{\nu_k} = 0 \end{cases}$$

Thus, we notice that under these conditions, the maximum value of β_{ij} is given by:

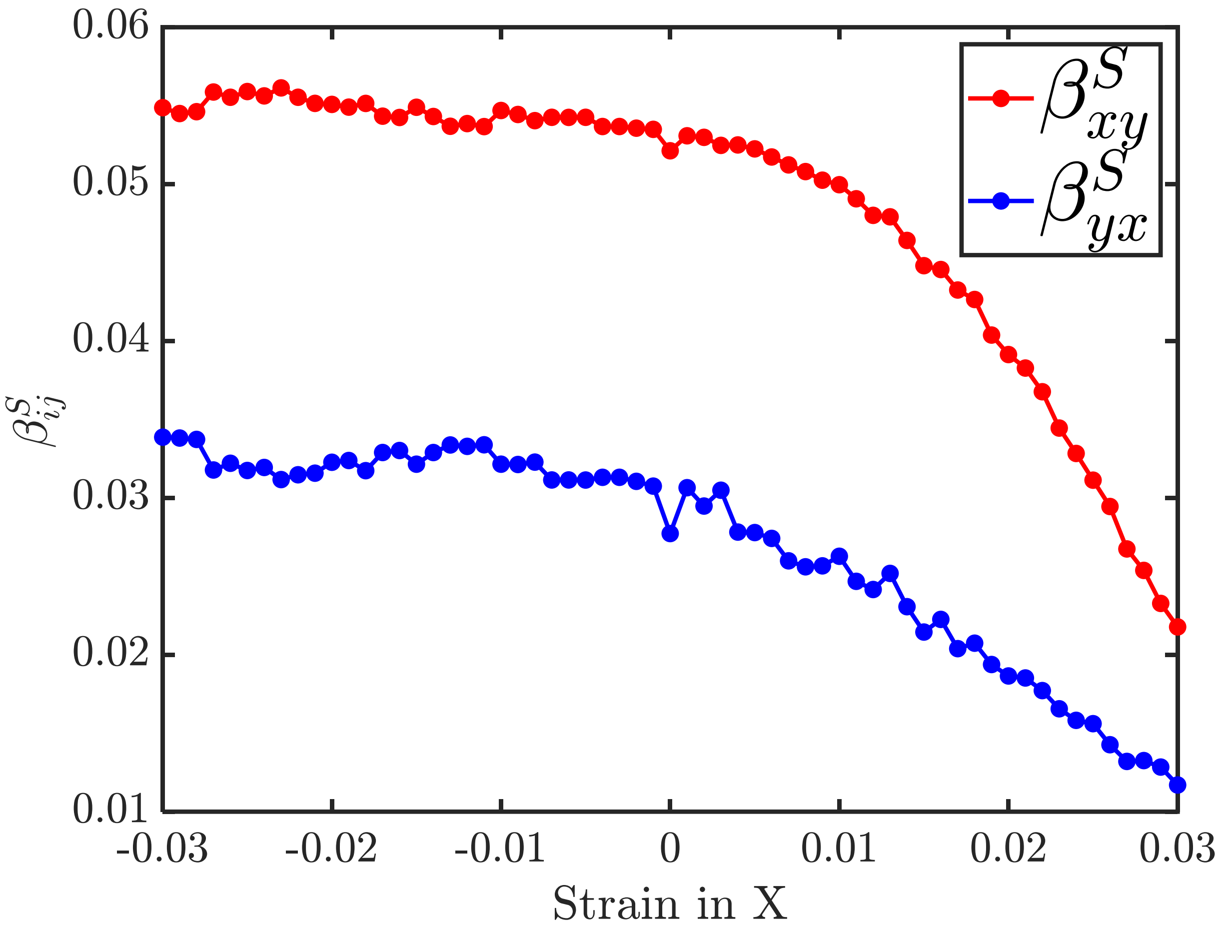
$$\beta_{ij} = \frac{9\sqrt{3}e^3 \operatorname{sgn}(C)}{32\pi^2 h^2} \frac{\nu_i^t}{\nu_j^t}$$

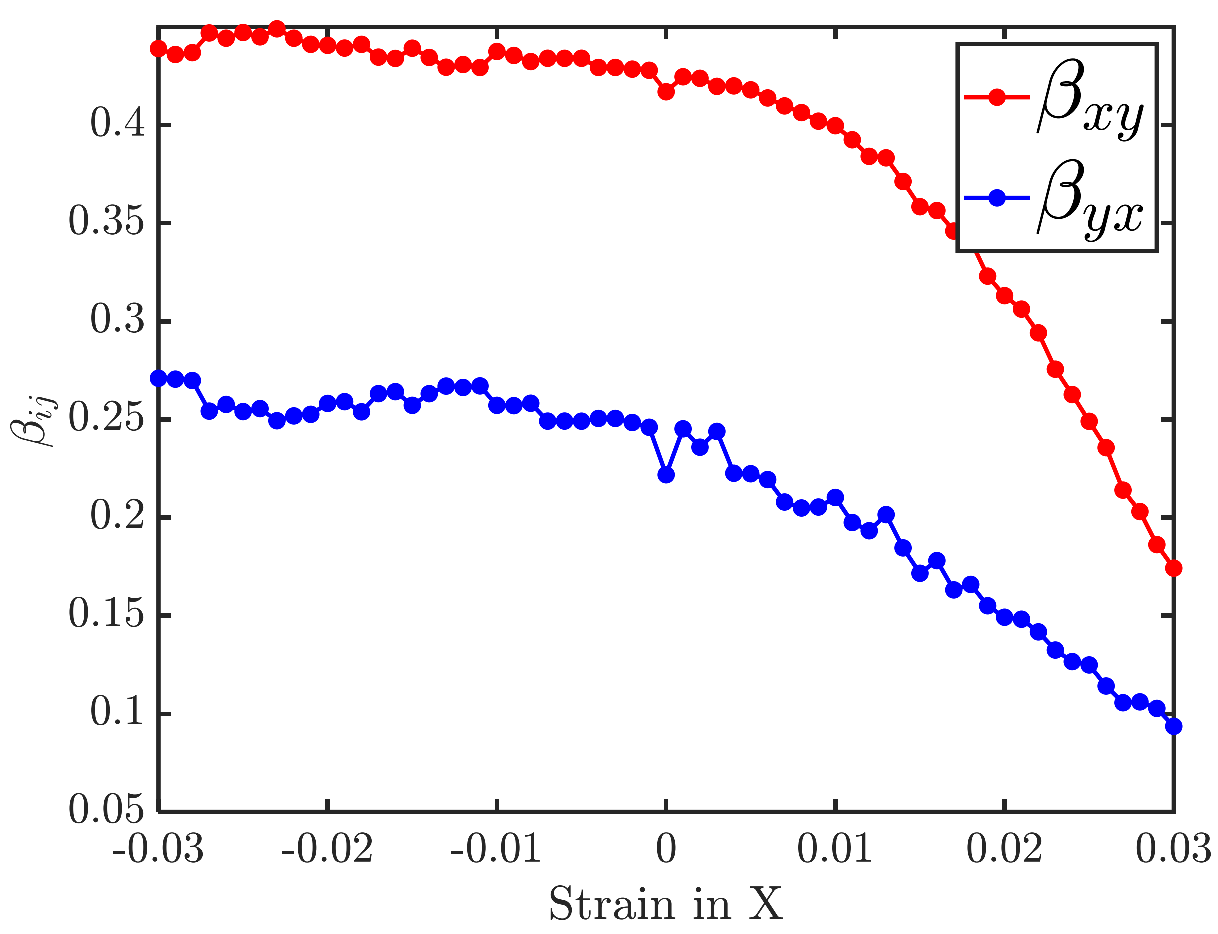
The maximum value of β_{xz} is profoundly affected by

$$\begin{cases} \dfrac{v_x^t}{v_x} = \dfrac{v_y^t}{v_y} \\ \dfrac{v_z^t}{v_z} = 0 \end{cases}$$

Thus, we notice that under these conditions, the maximum value of β_{xy} is given by:

$$\beta_{xy} = \frac{9\sqrt{3}e^3 \operatorname{sgn}(C)}{32\pi^2 h^2} \frac{v_x^t}{v_y^t}$$


0.06
0.05
0.04
0.03
0.02
0.01
β_{ij}^S
-0.03
-0.02
-0.01
0
0.01
0.02
0.03
Strain in X
β_{xy}^S
β_{yx}^S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0.35
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0.25
0.2
0.15
0.1
0.05
β_{ij}
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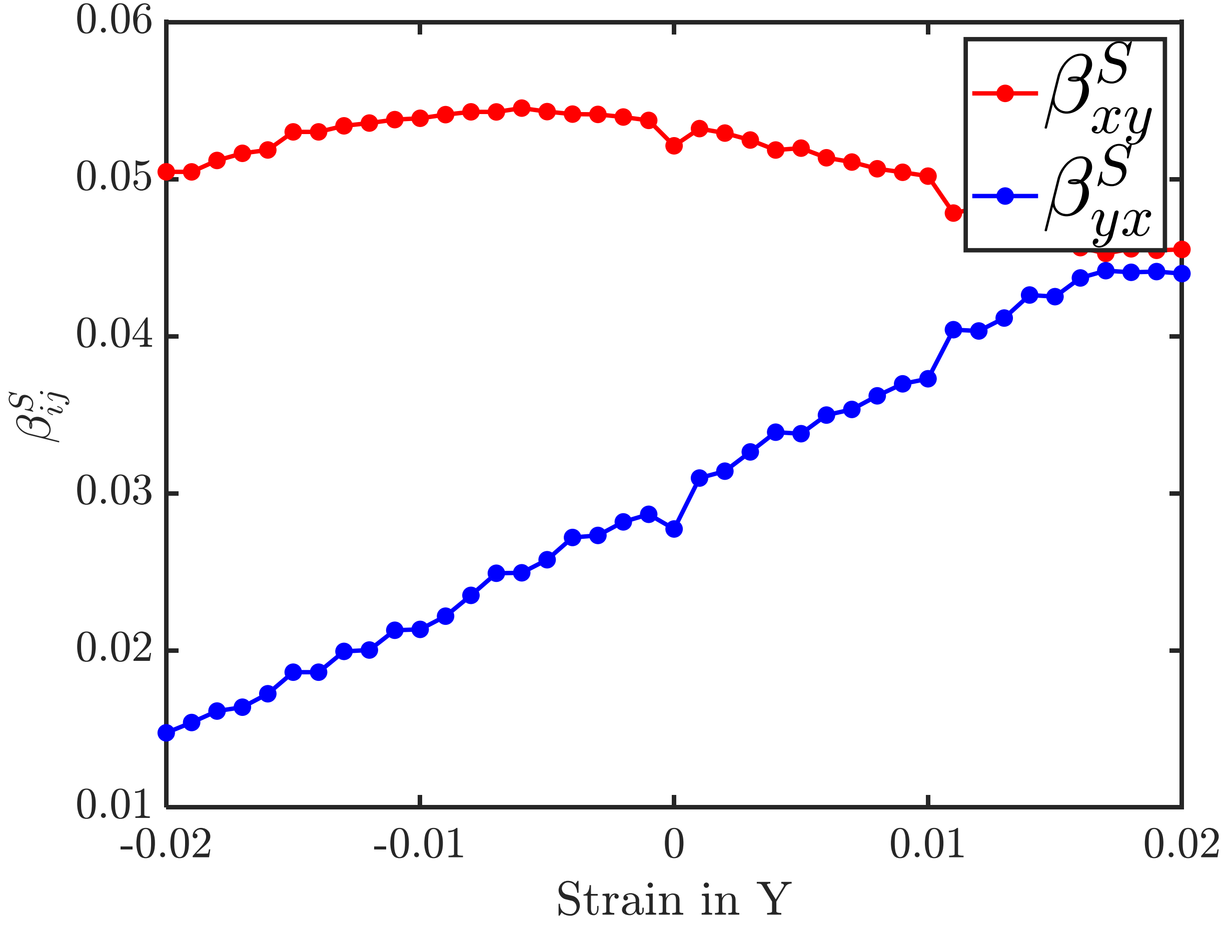
-0.02
-0.01
0
0.01
0.02
0.03
Strain in X
β_{xy}
β_{yx}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0
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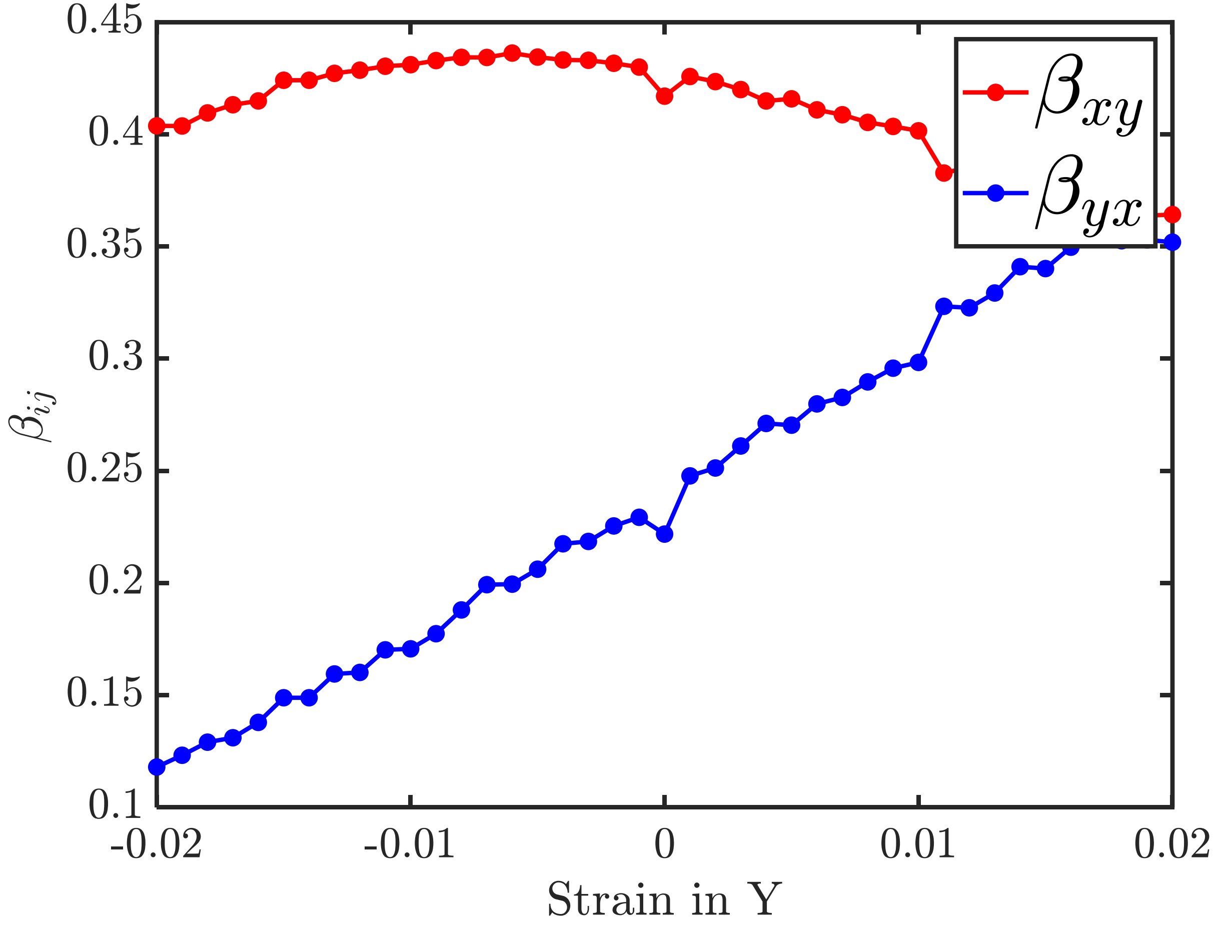
Strain in Y
β^S_{ij}
β^S_{xy}
β^S_{yx}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0.3
0.25
0.2
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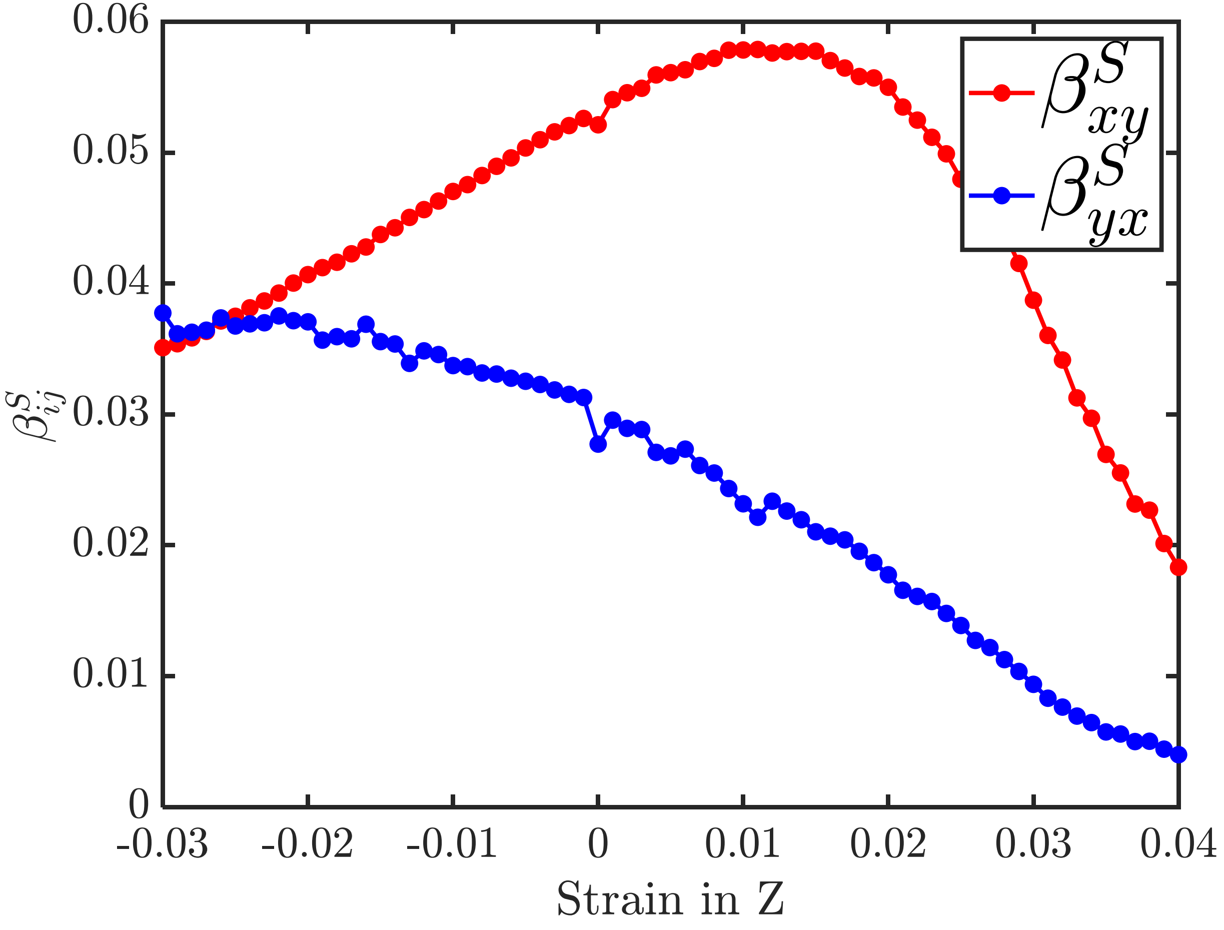
0
0.01
0.02
Strain in Y
β_{ij}
β_{xy}
β_{yx}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0.03
0.02
0.01
0
-0.03
-0.02
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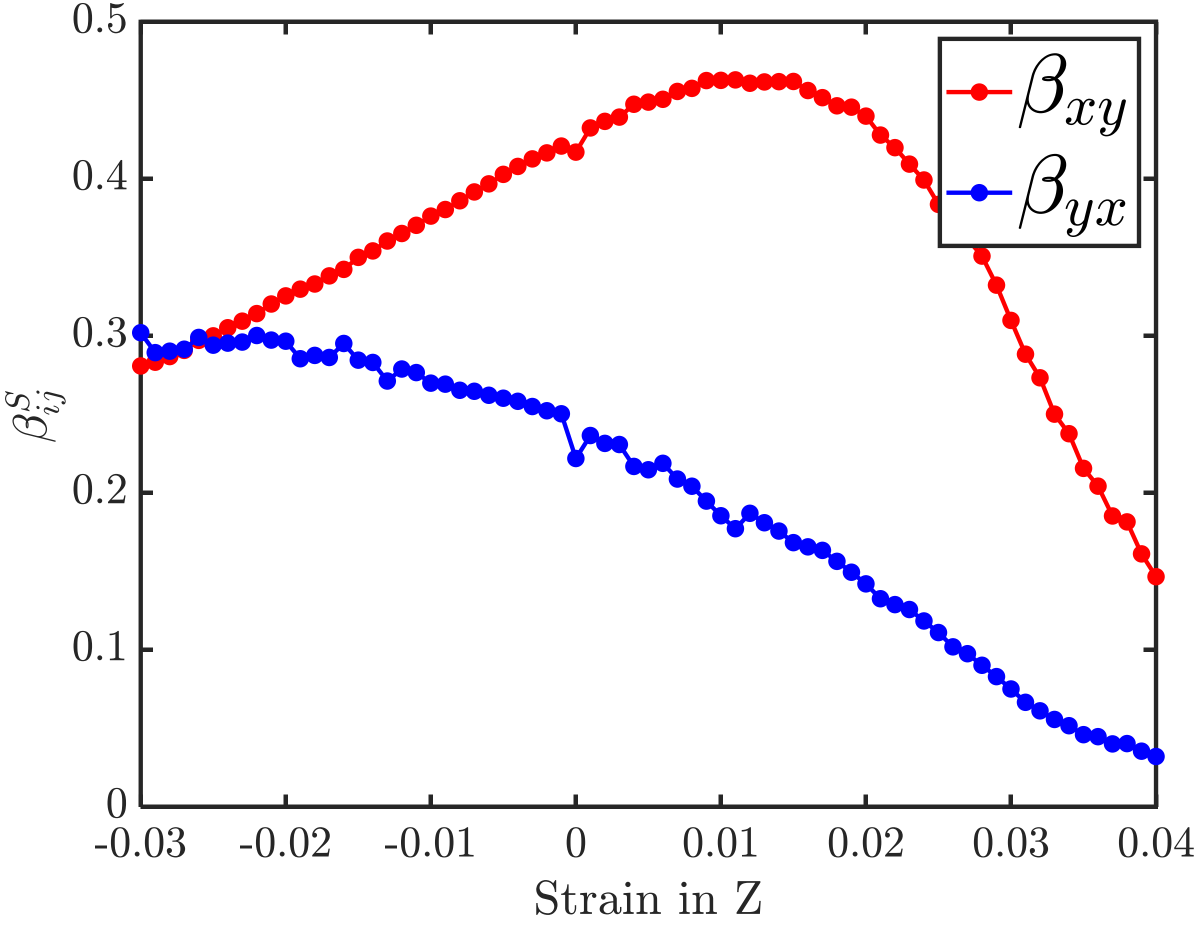
0
0.01
0.02
0.03
0.04
β_{ij}^{S}
Strain in Z
β_{xy}^{S}
β_{yx}^{S}


0.5
0.4
0.3
0.2
0.1
0
-0.03
-0.02
-0.01
0
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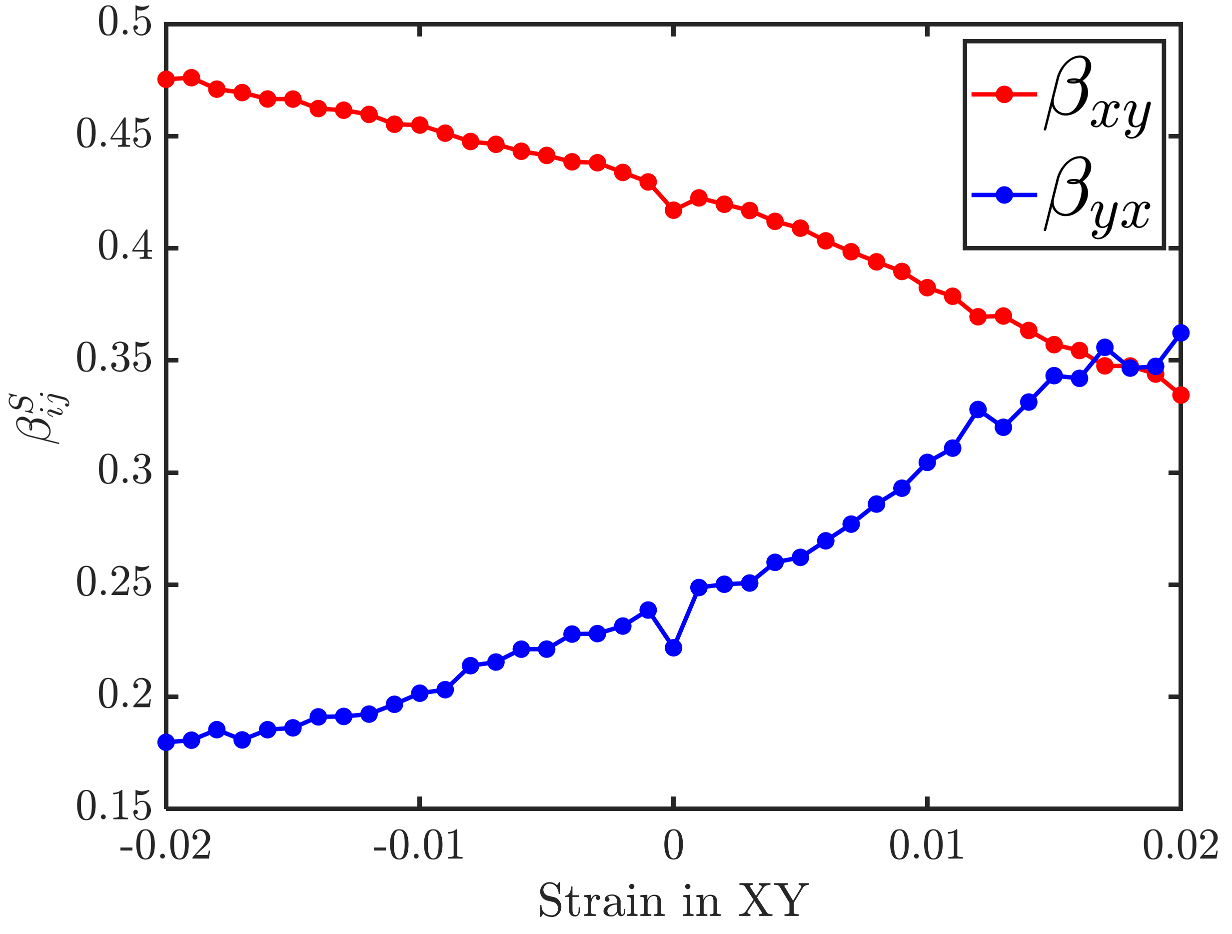
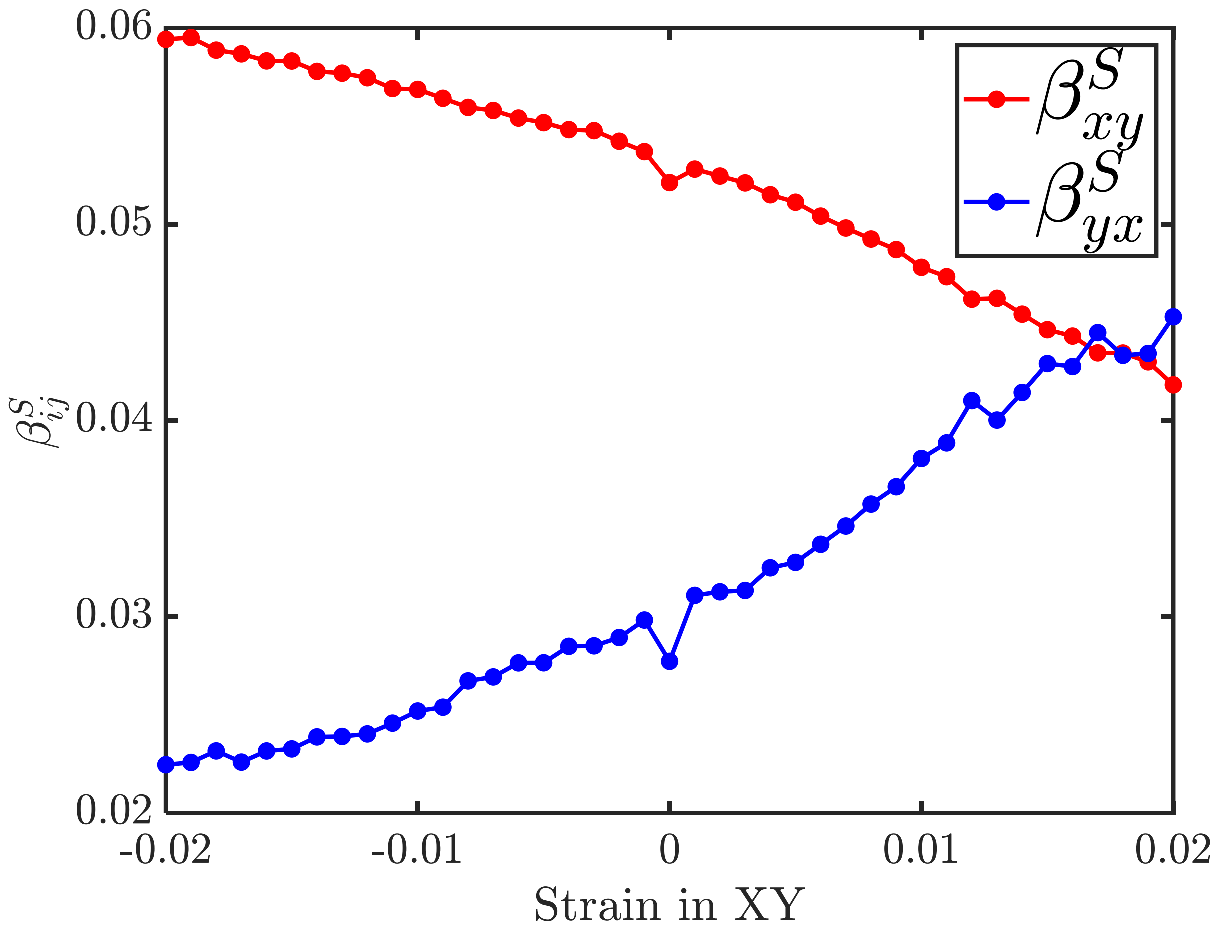
0.03
0.04
β_{ij}^{S}
Strain in Z
β_{xy}
β_{yx}

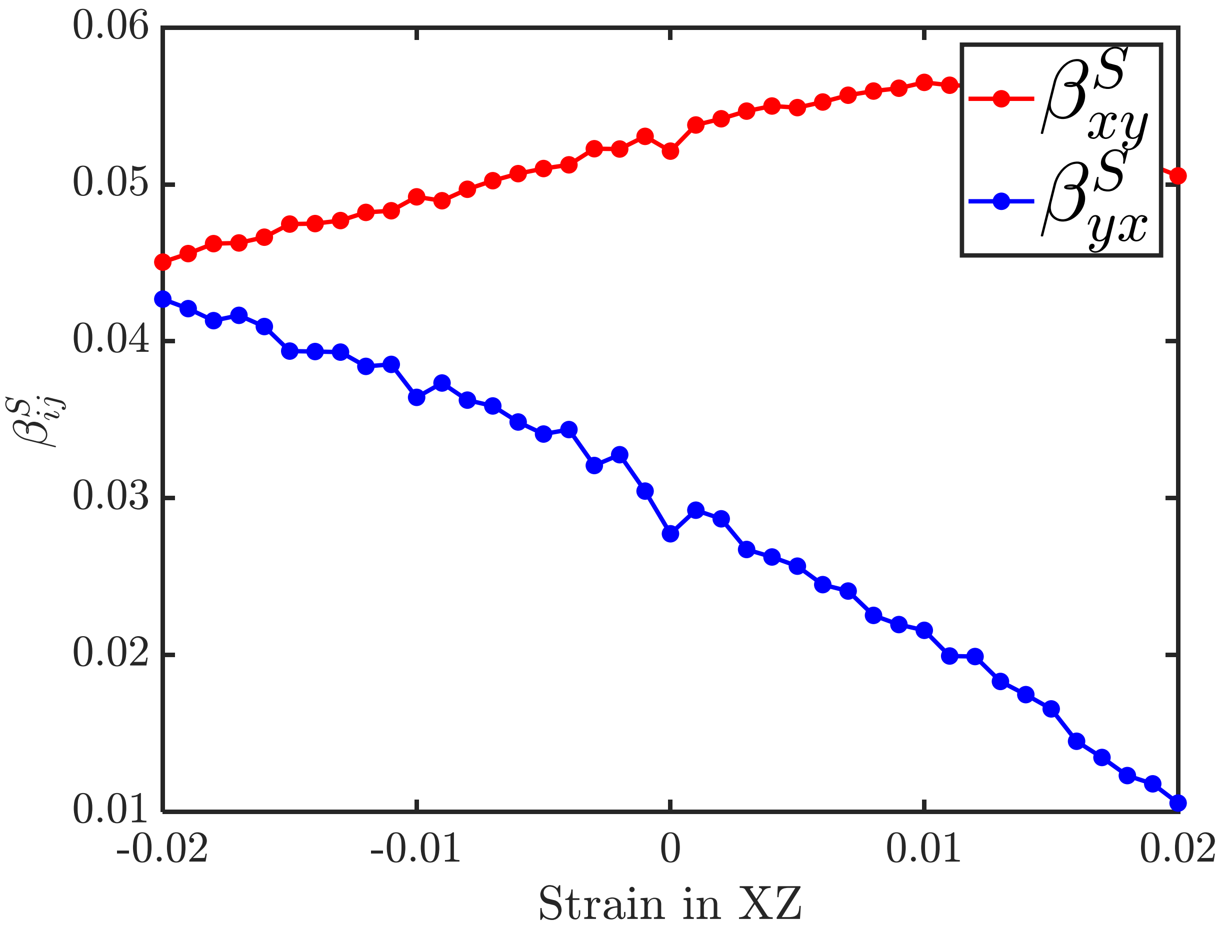
Strain in XY

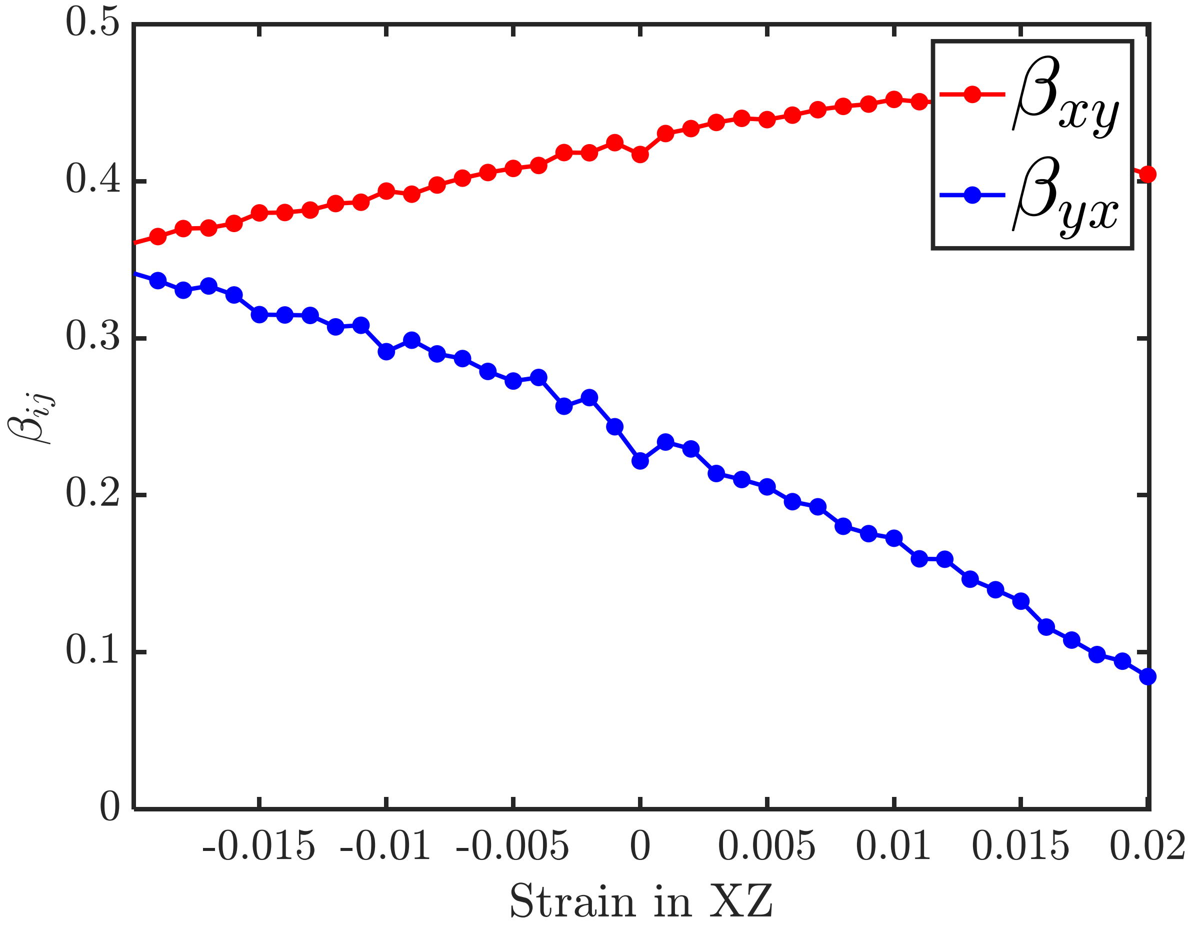


0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
-0.02
-0.01
0
0.01
0.02
Strain in XY
β_{ij}^S
β_{xy}
β_{yx}



0.06
0.05
0.04
0.03
0.02
-0.02
-0.01
0
0.01
0.02
Strain in XY
β_{ij}^S
β_{xy}^S
β_{yx}^S


0.06
0.05
0.04
0.03
0.02
0.01
β^S_{ij}
-0.02
-0.01
0
0.01
0.02
Strain in XZ
β^S_{xy}
β^S_{yx}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0.3
0.2
0.1
0
β_{ij}
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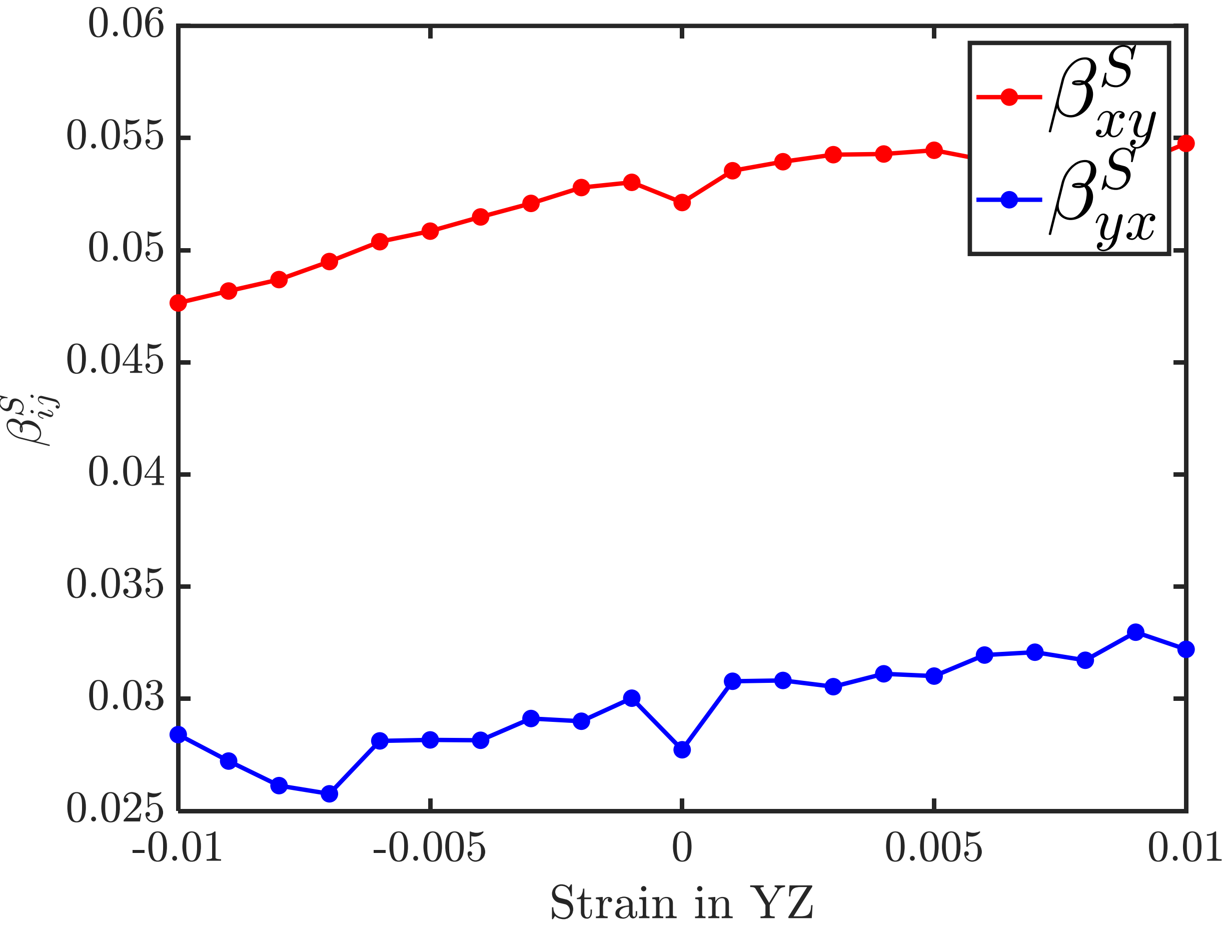
-0.01
-0.005
0
0.005
0.01
0.015
0.02
Strain in XZ
β_{xy}
β_{yx}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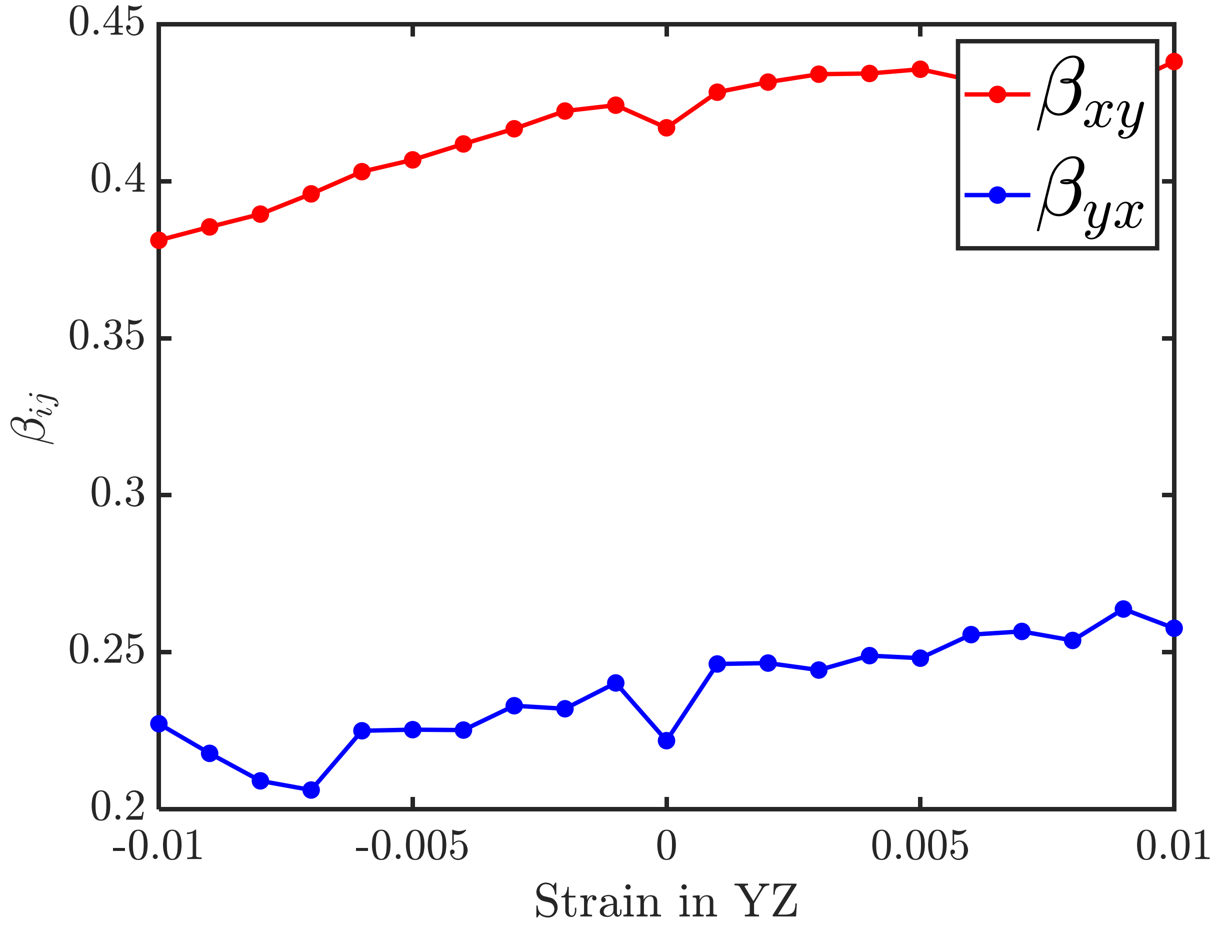
0.055
0.05
0.045
0.04
0.035
0.03
0.025
β_{ij}^S
-0.01
-0.005
0
0.005
0.01
Strain in YZ
β_{xy}^S
β_{yx}^S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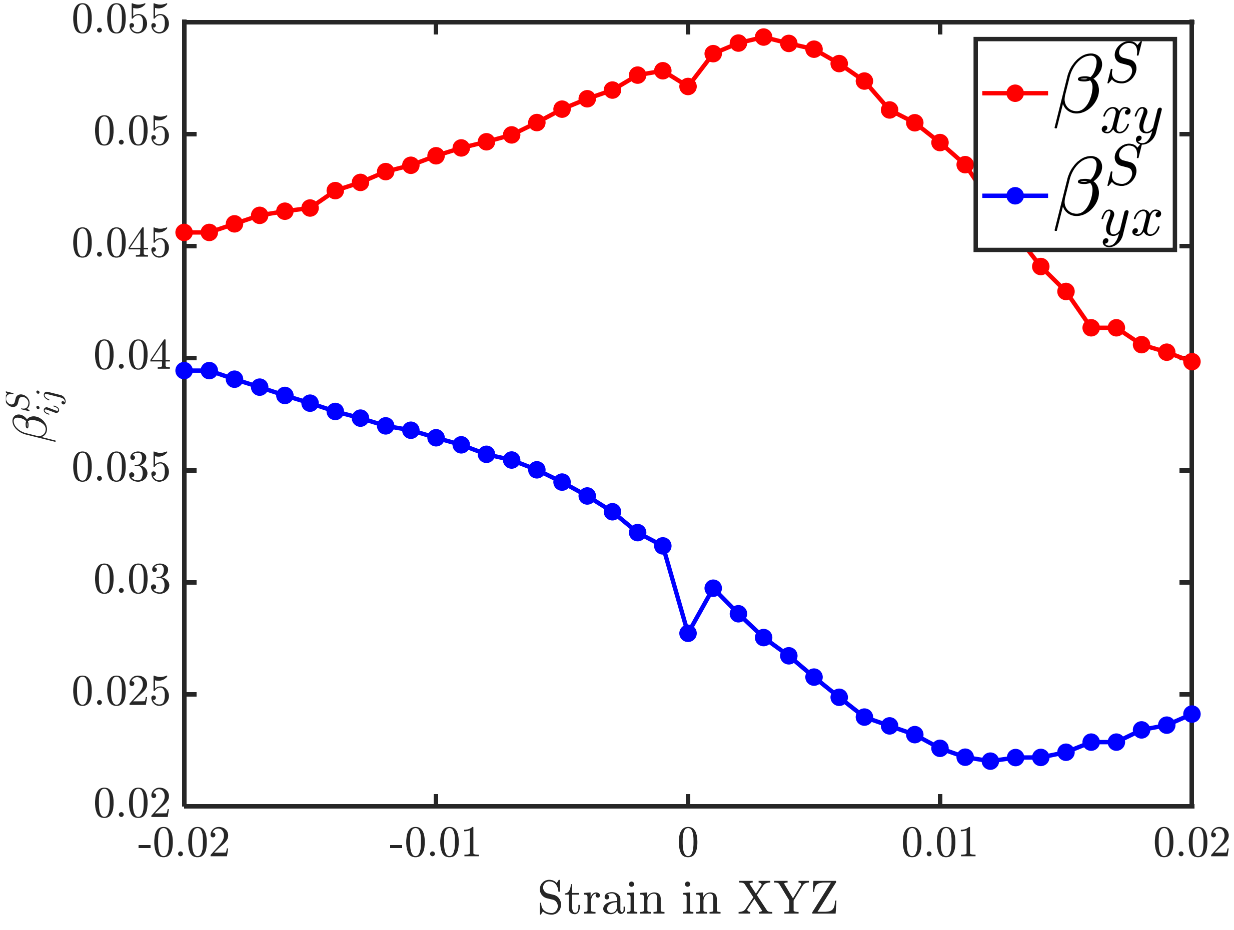
0.4
0.35
0.3
0.25
0.2
β_{ij}
-0.01
-0.005
0
0.005
0.01
Strain in YZ
β_{xy}
β_{yx}


0.055
0.05
0.045
0.04
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0.03
0.025
0.02
-0.02
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0
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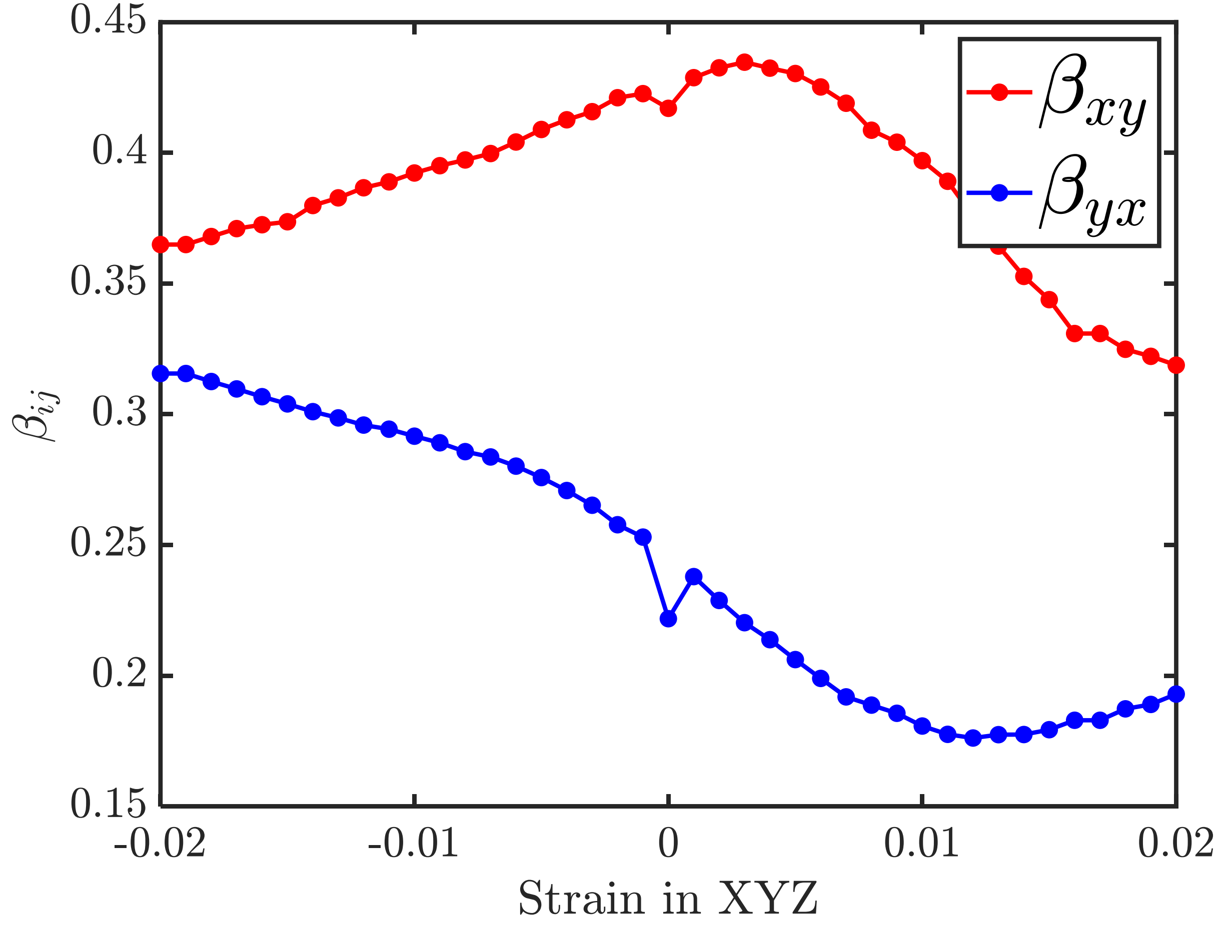
0.02
Strain in XYZ
β^S_{ij}
β^S_{xy}
β^S_{yx}


0.45
0.4
0.35
0.3
0.25
0.2
0.15
-0.02
-0.01
0
0.01
0.02
Strain in XYZ
β_{ij}
β_{xy}
β_{yx}