Green Lagrange Strain Tensor

We calculate the strain tensor if a unit cell with initial lattice parameter $a_1, b_1, c_1, \alpha_1, \beta_1$, and γ is changed to $a_2, b_2, c_2, \alpha_2, \beta_2$, and $\gamma + \Delta\gamma$.

For simplicity and 2D materials we take $\alpha_1 = 90°$, $\beta_1 = 90°$, and $c_1 = c_2$.

```
In[1]:= (*Initial cell array*)
C0 = {{a₁, 0, 0}, {b₁ Cos[γ], b₁ Sin[γ], 0}, {0, 0, c₁}};
C0 = Transpose[C0];
MatrixForm[C0]
```

Out[3]//MatrixForm=

$$\begin{pmatrix} a_1 & \cos[\gamma]\, b_1 & 0 \\ 0 & \sin[\gamma]\, b_1 & 0 \\ 0 & 0 & c_1 \end{pmatrix}$$

```
In[4]:= (*Final cell array*)
C1 = {{a₂, 0, 0}, {b₂ Cos[γ + Δγ], b₂ Sin[γ + Δγ], 0}, {0, 0, c₂}};
C1 = Transpose[C1];
MatrixForm[C1]
```

Out[6]//MatrixForm=

$$\begin{pmatrix} a_2 & \cos[\gamma + \Delta\gamma]\, b_2 & 0 \\ 0 & \sin[\gamma + \Delta\gamma]\, b_2 & 0 \\ 0 & 0 & c_2 \end{pmatrix}$$

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In[7]:= (*Deformation Gradient*)
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In[8]:= F = C1.Inverse[C0];
F // MatrixForm
```

Out[9]//MatrixForm=

$$\begin{pmatrix} \frac{a_2}{a_1} & -\frac{\cot[\gamma]\, a_2}{a_1} + \frac{\cos[\gamma+\Delta\gamma]\,\csc[\gamma]\, b_2}{b_1} & 0 \\ 0 & \frac{\csc[\gamma]\,\sin[\gamma+\Delta\gamma]\, b_2}{b_1} & 0 \\ 0 & 0 & \frac{c_2}{c_1} \end{pmatrix}$$

```
In[10]:= (*Green Lagrange Strain Tensor*)
GLDouble = (Transpose[F].F - IdentityMatrix[3]);
DisplayForm[1/2 MatrixForm[Simplify[GLDouble]]]
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Out[11]//DisplayForm=

$$\frac{1}{2}\begin{pmatrix} -1 + \frac{a_2^2}{a_1^2} & \frac{\csc[\gamma]\, a_2\,(-\cos[\gamma]\, a_2\, b_1 + \cos[\gamma+\Delta\gamma]\, a_1\, b_2)}{a_1^2\, b_1} & 0 \\ \frac{\csc[\gamma]\, a_2\,(-\cos[\gamma]\, a_2\, b_1 + \cos[\gamma+\Delta\gamma]\, a_1\, b_2)}{a_1^2\, b_1} & -1 + \frac{\csc[\gamma]^2\,\sin[\gamma+\Delta\gamma]^2\, b_2^2}{b_1^2} + \left(\frac{\cot[\gamma]\, a_2}{a_1} - \frac{\cos[\gamma+\Delta\gamma]\,\csc[\gamma]\, b_2}{b_1}\right)^2 & 0 \\ 0 & 0 & -1 + \frac{c_2^2}{c_1^2} \end{pmatrix}$$

In[12]:= (*For Simplicity let use also take $\gamma_1 = \frac{\pi}{2}$ *)

Clear[{γ}];

$\gamma = \dfrac{\pi}{2}$;

DisplayForm$\left[\dfrac{1}{2}$ MatrixForm[Simplify[GLDouble]]$\right]$

Out[14]//DisplayForm=

$$\frac{1}{2}\begin{pmatrix} -1 + \dfrac{a_2^2}{a_1^2} & -\dfrac{\text{Sin}[\Delta\gamma]\, a_2\, b_2}{a_1\, b_1} & 0 \\[2ex] -\dfrac{\text{Sin}[\Delta\gamma]\, a_2\, b_2}{a_1\, b_1} & -1 + \dfrac{b_2^2}{b_1^2} & 0 \\[2ex] 0 & 0 & -1 + \dfrac{c_2^2}{c_1^2} \end{pmatrix}$$