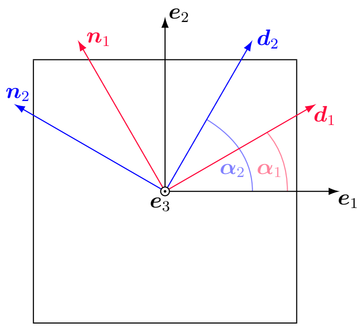
Exercise 12

1. Crystal plasticity

Problem

We consider a rigid-plastic single crystal with two slip systems ($\boldsymbol{d}_1$, $\boldsymbol{n}_1$ and $\boldsymbol{d}_2$, $\boldsymbol{n}_2$), subjected to an isochoric deformation, plane in e_3-direction, realized by a constant velocity gradient. The initial lattice ($t = 1$) corresponds to the reference lattice.



Task

Determine the system of equations which governs the shear in both slip systems and the lattice rotation. Give a solution for a symmetric deformation gradient $\boldsymbol{L}$. Examine the system for the case $\alpha_2 = \alpha_1 + {}^{\pi}/_{2}$. Solve the system for a shear test ($\boldsymbol{L} = \dot{\gamma}_0\, \boldsymbol{e}_1 \otimes \boldsymbol{e}_2$) and an isochoric tension test ($\boldsymbol{L} = \dot{\gamma}_0(\boldsymbol{e}_1 \otimes \boldsymbol{e}_1 - \boldsymbol{e}_2 \otimes \boldsymbol{e}_2)$) numerically for different angles α_1 and α_2 and discuss the results.

Solution

The overall deformation gradient is given by

$$\boldsymbol{F} = \boldsymbol{F}_\mathrm{e} \cdot \boldsymbol{P}^{-1} \, .$$

By demanding rigid-plastic-material behaviour, the elastic part must be $\boldsymbol{F}_\mathrm{e} \in \mathscr{O}rth^+$. The deformation gradient is linked to the velocity gradient by

$$\boldsymbol{L} = \dot{\boldsymbol{F}} \cdot \boldsymbol{F}^{-1} \, .$$

The rate of slip is linked to the rate of plastic transformation by

$$-\boldsymbol{P}^{-1} \cdot \dot{\boldsymbol{P}} = \sum_{i=1}^{n} \dot{\gamma}_i\, \boldsymbol{d}_i \otimes \boldsymbol{n}_i$$

where i runs over all slip systems. In this equation, the lattice vectors are constant reference vectors. We can put this four equations together by taking the time derivative of $\boldsymbol{F}$, plugging it into $\boldsymbol{L} = \dot{\boldsymbol{F}} \cdot \boldsymbol{F}^{-1}$, and set $\boldsymbol{F}_\mathrm{e} = \boldsymbol{Q} \in \mathscr{O}rth$, which gives

$$\boldsymbol{L} = \dot{\boldsymbol{Q}} \cdot \boldsymbol{Q}^\top + \boldsymbol{Q} \cdot (\boldsymbol{P}^{-1})^{\cdot} \cdot \boldsymbol{P} \cdot \boldsymbol{Q}^\top \, .$$

By considering

$$\dot{\boldsymbol{I}} = \boldsymbol{0} = (\boldsymbol{P}^{-1} \cdot \boldsymbol{P})^{\cdot} = (\boldsymbol{P}^{-1})^{\cdot} \cdot \boldsymbol{P} + \boldsymbol{P}^{-1} \cdot \dot{\boldsymbol{P}}$$

we find that

$$(\boldsymbol{P}^{-1})^{\cdot} \cdot \boldsymbol{P} = -\boldsymbol{P}^{-1} \cdot \dot{\boldsymbol{P}} = \sum_{i=1}^{n} \dot{\gamma}_i\, \boldsymbol{d}_i \otimes \boldsymbol{n}_i$$

so that $\boldsymbol{L}$ becomes

$$\boldsymbol{L} = \dot{\boldsymbol{Q}} \cdot \boldsymbol{Q}^\top + \boldsymbol{Q} \cdot \sum_{i=1}^{n} \dot{\gamma}_i \, \boldsymbol{d}_i \otimes \boldsymbol{n}_i \cdot \boldsymbol{Q}^\top \ .$$

The lattice spin must take place in $\boldsymbol{e}_3$-plane. Thus we can parametrize $\boldsymbol{Q} = Q_{ij} \boldsymbol{e}_i \otimes \boldsymbol{e}_j$ by

$$[Q_{ij}] = \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \ .$$

With this we get easily $\dot{\boldsymbol{Q}} \cdot \boldsymbol{Q}^\top$.

$$[\dot{Q}_{ij} Q_{ji}] = \begin{bmatrix} 0 & \dot{\phi} & 0 \\ -\dot{\phi} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \ .$$

When introducing the abbreviations

$$c_1 = \cos(\alpha_1) \qquad s_1 = \sin(\alpha_1)$$
$$c_2 = \cos(\alpha_2) \qquad s_2 = \sin(\alpha_2)$$

we can give $\boldsymbol{d}_i$ and $\boldsymbol{n}_i$ with respect to the constant basis $\boldsymbol{e}_i$.

$$\begin{aligned} \boldsymbol{d}_i &= c_i \boldsymbol{e}_1 + s_i \boldsymbol{e}_2 \\ \boldsymbol{n}_i &= -s_i \boldsymbol{e}_1 + c_i \boldsymbol{e}_2 \end{aligned}$$

Putting all together, we can give the components of $\boldsymbol{L}$ with respect to the basis $\boldsymbol{e}_i \otimes \boldsymbol{e}_j$. Hereby it is sufficient to consider the upper left 2×2 matrix.

$$\begin{bmatrix} L_{11} & L_{12} \\ L_{21} & -L_{11} \end{bmatrix} = \begin{bmatrix} 0 & \dot{\phi} \\ -\dot{\phi} & 0 \end{bmatrix} \begin{bmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{bmatrix} \left(\dot{\gamma}_1 \begin{bmatrix} -s_1 c_1 & c_1^2 \\ -s_1^2 & s_1 c_1 \end{bmatrix} + \dot{\gamma}_2 \begin{bmatrix} -s_2 c_2 & c_2^2 \\ -s_2^2 & s_2 c_2 \end{bmatrix} \right) \begin{bmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{bmatrix}$$

Here we have considered that $\boldsymbol{L}$ must be deviatoric and plane in the $\boldsymbol{e}_3$-plane, i.e., there remain only three independent components. It becomes evident that we can not consider more than two slip systems, otherwise we would have more than three functions to be determined (now $\phi(t)$, $\gamma_1(t)$, and $\gamma_2(t)$), but still only three equations[1]. The latter equation is summarized as follows.

$$\begin{bmatrix} L_{11} & L_{12} \\ L_{21} & -L_{11} \end{bmatrix} = \begin{bmatrix} -\frac{1}{2}(\dot{\gamma}_1 \sin(2(\alpha_1 - \phi)) + (\dot{\gamma}_2 \sin(2(\alpha_2 - \phi))) & \dot{\gamma}_1 \cos^2(\alpha_1 - \phi) + \dot{\gamma}_2 \cos^2(\alpha_2 - \phi) + \dot{\phi} \\ -\dot{\gamma}_1 \sin^2(\alpha_1 - \phi) - \dot{\gamma}_2 \sin^2(\alpha_2 - \phi) - \dot{\phi} & \frac{1}{2}(\dot{\gamma}_1 \sin(2(\alpha_1 - \phi)) + (\dot{\gamma}_2 \sin(2(\alpha_2 - \phi))) \end{bmatrix}$$

We immediately note that the right-hand side 22-component is the negative of the right-hand side 11-component, as it is the case on the left-hand side., i.e., comparing the coefficients 11 and 22 gives the same equation. We have, indeed, only three independent equations. The right-hand side is traceless due to the fact that shear deformations (and superpositions of shear deformations) are isochoric.

We need a little more time to note what happens in the case $\alpha_2 = \alpha_1 + \pi/2$. With the relations

$$\cos(x + \pi/2) = -\sin(x) \qquad \sin(x + \pi/2) = \cos(x)$$
$$\sin(x + \pi/2) = -\sin(x) \qquad \sin^2(x) + \cos^2(x) = 1$$

[1] This is known as the Taylor problem. In three dimensions, a deviatoric $\boldsymbol{L}$ has eight independent components. A general $\boldsymbol{Q}$ is parameterized by three angles, which leaves five linear independent slip systems. In general, a crystal lattice has more than five slip systems, which leaves the problem as it is considered here with a variety of solutions. The problem of uniqueness is overcome by taking into account elastic strains, which give rise to stresses (material law), which are used to determine a Schmid stress in each slip system. By postulating a slip rate-stress relation (more material law), the plastic deformation can be uniquely related to the stress state, which is uniquely related to the actual state of plastic and elastic deformation.

we can reformulate the latter matrix equation for the case $\alpha_2 = \alpha_1 + {}^{\pi}\!/\!_2$ to

$$\begin{bmatrix} L_{11} & L_{12} \\ L_{21} & -L_{11} \end{bmatrix} = \begin{bmatrix} -\frac{1}{2}\sin(2(\alpha_1-\phi))(\dot\gamma_1-\dot\gamma_2) & \cos^2(\alpha_1-\phi)(\dot\gamma_1-\dot\gamma_2)+\dot\phi+\dot\gamma_2 \\ -\sin^2(\alpha_1-\phi)-(\dot\gamma_1-\dot\gamma_2)-\dot\phi-\dot\gamma_2 & \frac{1}{2}\sin(2(\alpha_1-\phi))(\dot\gamma_1-\dot\gamma_2) \end{bmatrix}$$

One now notes that we can substitute $\dot\gamma_1 - \dot\gamma_2 =: \Delta\dot\gamma$ and $\dot\phi + \dot\gamma_2 =: \dot\phi^*$, which leaves a system of three differential equations with effectively two undetermined functions. It is not to expect that we can find two functions that satisfy three independent equations. Thus, we must exclude the case $\alpha_2 = \alpha_1 + {}^{\pi}\!/\!_2$ from our considerations.

Analytical solution for symmetric $\boldsymbol{L}$

Considering the the skew part of our original matrix equation for $\boldsymbol{L} = \boldsymbol{D} + \boldsymbol{W}$ gives

$$W_{12} = \dot\phi + \tfrac{1}{2}(\dot\gamma_1 + \dot\gamma_2).$$

By considering the symmetric part we have

$$\boldsymbol{D} = \frac{\dot\gamma_1}{2}\boldsymbol{Q}\cdot(\boldsymbol{d}_1\otimes\boldsymbol{n}_1+\boldsymbol{n}_1\otimes\boldsymbol{d}_1)\cdot\boldsymbol{Q}^\top + \frac{\dot\gamma_2}{2}\boldsymbol{Q}\cdot(\boldsymbol{d}_2\otimes\boldsymbol{n}_2+\boldsymbol{n}_2\otimes\boldsymbol{d}_2)\cdot\boldsymbol{Q}^\top$$

$\boldsymbol{D}$ is symmetric and traceless, hence there are two independent components D_{11} and D_{12}. Presuming that $\boldsymbol{d}_1\otimes\boldsymbol{n}_1+\boldsymbol{n}_1\otimes\boldsymbol{d}_1$ and $\boldsymbol{d}_2\otimes\boldsymbol{n}_2+\boldsymbol{n}_2\otimes\boldsymbol{d}_2$ are linearly independent, the latter is a linear system for $\dot\gamma_{1,2}$. Its solutions are

$$\begin{aligned}\dot\gamma_1 &= -\frac{2}{\sin(2(\alpha_1-\alpha_2))}\left(D_{11}\cos(2(\alpha_2-\phi))+D_{12}\sin(2(\alpha_2-\phi))\right)\\ \dot\gamma_2 &= \quad\frac{2}{\sin(2(\alpha_1-\alpha_2))}\left(D_{11}\cos(2(\alpha_1-\phi))+D_{12}\sin(2(\alpha_1-\phi))\right).\end{aligned}$$

We note that in case of $\alpha_2 - \alpha_1 = n\,{}^{\pi}\!/\!_2$, $n \in \mathbb{Z}$, the solution is not defined. We can insert the latter two equations into W_{12}, which gives an ODE only for ϕ.

$$W_{12} = \frac{1}{\sin(\alpha_1+\alpha_2)}\left(D_{12}\cos(\alpha_1+\alpha_2-2\phi) - D_{11}\sin(\alpha_1+\alpha_2-2\phi)\right) + \dot\phi$$

This ODE can be simplified considerably by noting that we can use trigonometric functions to parameterize the set of possible deviatoric $\boldsymbol{D}$ in the subsequent manner.

$$[D_{ij}] = \frac{D}{\sqrt{2}}\begin{bmatrix}\cos\delta & \sin\delta \\ \sin\delta & -\cos\delta\end{bmatrix}$$

with $D = \|\boldsymbol{D}\|$ and δ as parameterization. This means, we change the independent components D_{11} and D_{22} for $\|\boldsymbol{D}\|$ and δ. After employing a trigonometric relation, the ODE reads as follows.

$$W_{12} = -K\,\sin(\alpha_1+\alpha_2-\delta-2\phi)+\dot\phi \qquad K = \frac{D}{\sqrt{2}\cos(\alpha_1-\alpha_2)}$$

One notes that in case of $\alpha_2 - \alpha_1 = {}^{\pi}\!/\!_2 + n\pi$, $n \in \mathbb{Z}$, K is not defined. The latter ODE can be solved for symmetric and constant $\boldsymbol{L}$, i.e., for $W_{12} = 0$ and constant K:

$$\dot\phi = K\,\sin(\alpha_1+\alpha_2-\delta-2\phi)$$

Introducing $\beta = \alpha_1+\alpha_2-\delta-2\phi$ and consequently $\dot\phi = -{}^{\dot\beta}\!/\!_2$ we have

$$\begin{aligned}\dot\beta &= -2K\,\sin(\beta)\\ \frac{\mathrm{d}\beta}{\sin(\beta)} &= -2K\,\mathrm{d}t\,.\end{aligned}$$

Integration gives:

$$\begin{aligned}\ln(\tan(\beta/2)) &= -2Kt + C\\ \phi &= -\arctan(\exp(-2Kt+C)) + \frac{\alpha_1+\alpha_2-\delta}{2}\end{aligned}$$

C is determined from initial condition $\phi(0) = 0$, i.e.,

$$C = \ln\left(\tan\left(\frac{\alpha_1+\alpha_2-\delta}{2}\right)\right)$$

We can substitute ϕ in

$$\begin{aligned}\dot{\gamma}_1 &= -\sqrt{2}D\,\frac{\cos(2\alpha_2-\delta-2\phi)}{\sin(2(\alpha_1-\alpha_2))}\\ \dot{\gamma}_2 &= \quad\sqrt{2}D\,\frac{\cos(2\alpha_1-\delta-2\phi)}{\sin(2(\alpha_1-\alpha_2))}\end{aligned}$$

which - after invoking some trigonometric relations - gives

$$\begin{aligned}\dot{\gamma}_1 &= -\frac{K}{\sin(\alpha_1-\alpha_2)}\,\cos\left(\alpha_1-\alpha_2-2\,\mathrm{arccot}\left(\exp(2Kt)\cot\left(\frac{\alpha_1+\alpha_2-\delta}{2}\right)\right)\right)\\ \dot{\gamma}_2 &= \quad\frac{K}{\sin(\alpha_1-\alpha_2)}\,\cos\left(\alpha_1-\alpha_2+2\,\mathrm{arccot}\left(\exp(2Kt)\cot\left(\frac{\alpha_1+\alpha_2-\delta}{2}\right)\right)\right)\ .\end{aligned}$$

Luckily, the latter can be integrated, which gives solutions for γ_1 and γ_2:

$$\begin{aligned}\gamma_1 &= a + b + \tilde{\gamma}_1\\ \gamma_2 &= a - b + \tilde{\gamma}_1\ ,\end{aligned}$$

wherein

$$\begin{aligned}a &= -\arctan\left(\mathrm{e}^{2Kt}\cot\left(\tfrac{1}{2}(\alpha_1+\alpha_2-\delta)\right)\right)\\ b &= \quad\tfrac{1}{2}\cot(\alpha_1-\alpha_2)\left(2Kt - \ln\left(1+\mathrm{e}^{4Kt}+(\mathrm{e}^{4Kt}-1)\cos(\alpha_1+\alpha_2-\delta)\right)\right)\ .\end{aligned}$$

From the initial conditions $\gamma_i = 0$ at $t = 0$ we obtain $\tilde{\gamma}_i$

$$\begin{aligned}\tilde{\gamma}_1 &= -\tilde{a} - \tilde{b}\\ \tilde{\gamma}_2 &= -\tilde{a} + \tilde{b}\ ,\end{aligned}$$

where

$$\begin{aligned}\tilde{a} &= -\arctan\left(\cot\left(\frac{\alpha_1+\alpha_2-\delta}{2}\right)\right)\\ \tilde{b} &= -\ln(2)\frac{\cot(\alpha_1-\alpha_2)}{2}\ .\end{aligned}$$

We can examine the behaviour as t tends to infinity: $\exp(Kt + C)$ tends either to 0 or to ∞, depending on the sign of K, which means that

(1) ϕ tends to $(\alpha_1+\alpha_2-\delta)/2$ or $(\alpha_1+\alpha_2-\delta-\pi)/2$

A little bit of geometric consideration shows that ϕ always tends to the bisection of the smaller one of the angles that $\boldsymbol{d}_1$ and $\pm\boldsymbol{d}_2$ form. Since ϕ tends to stationary value, it follows from the equations for $\dot{\gamma}_i$ given above that

(2) $\dot{\gamma}_i$ tend to constant values of different sign but the same absolute value, thus γ_i approach a linear function, and

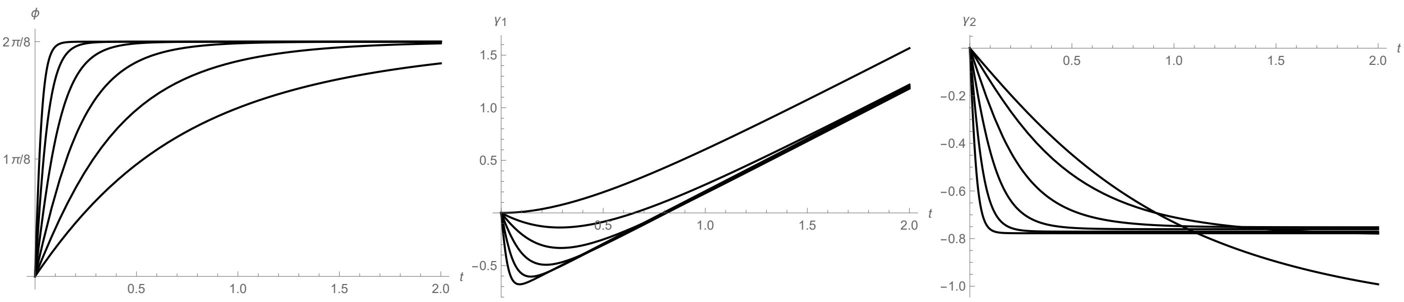
(3) the influence of δ on $\dot{\gamma}_i$ tends to zero as t tends to infinity.

The analytical results have been compared to numerical results, which are obtained easily by employing a numerical time integration scheme, and found to practically coincide. Thus, the analytical findings are very likely to be correct. However, we are due to the assumption that $\boldsymbol{L} = \boldsymbol{D}$ not able to give results for a simple shear test analytically, und must resort to numerical approximations.

Shear and elongation test

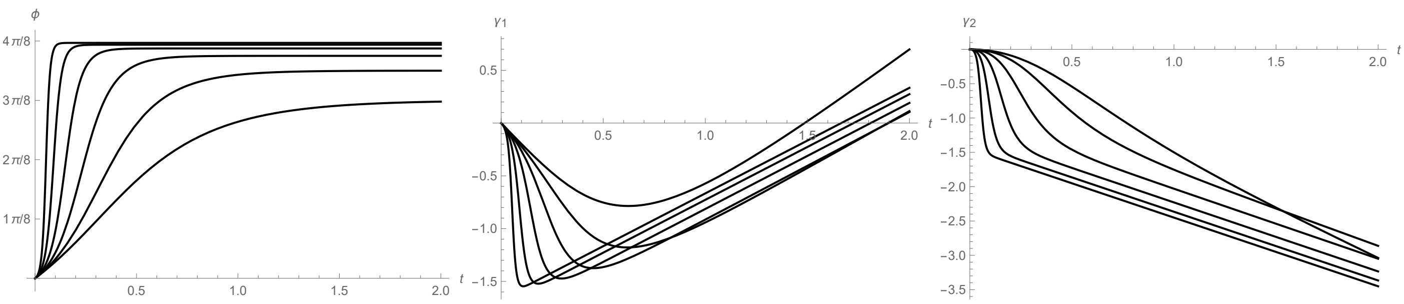
Let us have a look at the numerical solution for different conditions. We take $\alpha_1 = {}^{\pi}/_{4}$ as constant, and $\alpha_2 = \alpha_1 + {}^{\pi}/_{2}(1 - {}^{1}/_{2^i})$. By this, we can examine the behaviour of the system as $\alpha_2 \to \alpha_1 + {}^{\pi}/_{2}$ by taking $i \to \infty$. The MMA code given at the end of this sheet solves the system numerically and plots the solutions. It can be used for both tests.

Here we start with the results for the shear test $\boldsymbol{L} = \dot{\gamma}_0\, \boldsymbol{e}_1 \otimes \boldsymbol{e}_2$ with $\dot{\gamma}_0 = {}^{1}/_{\mathrm{s}}$ for different $\alpha_2 (i = 1 \ldots 6)$.



The results indicate that during the shear test, the lattice undergoes a rotation which tends asymptotically to an absolute rotation angle of ${}^{\pi}/_{4}$. This rotation leaves slip system 1 perfectly aligned to accommodate the global shear deformation, i.e., the spatial lattice vectors $\boldsymbol{Q} \cdot \boldsymbol{d}_1 \to \boldsymbol{e}_1$ and $\boldsymbol{Q} \cdot \boldsymbol{n}_1 \to \boldsymbol{e}_2$. This tendency is more pronounced as $\alpha_2 \to \alpha_1 + {}^{\pi}/_{2}$.

The following results are for the elongation test $\boldsymbol{L} = \dot{\gamma}_0 (\boldsymbol{e}_1 \otimes \boldsymbol{e}_1 - \boldsymbol{e}_2 \otimes \boldsymbol{e}_2)$ with $\dot{\gamma}_0 = {}^{1}/_{\mathrm{s}}$ for different $\alpha_2 (i = 1 \ldots 6)$.



The results indicate, that during the elongation test, the lattice undergoes a rotation which tends asymptotically to an absolute rotation angle of ${}^{1}/_{2}(\alpha_1 + \alpha_2)$. This rotation leaves the slip systems aligned symmetrically with respect to the elongation direction, i.e., both slip systems contribute equally to the imposed elongation test. This tendency is more pronounced as $\alpha_2 \to \alpha_1 + {}^{\pi}/_{2}$.

One can imagine that, since this toy problem is hardly manageable analytically, a real crystal (with more slip systems, employing elasticity, Schmid law and flow rule to avoid Taylor problem), or even a polycrystal (grain interaction, solution of the boundary value problem) requires numerical methods or strong restrictions.

MMA code

```
Remove["Global`*"]

(* initialize empty lists for the plots *)

plotsphi = {};
plotsgamma1 = {};
plotsgamma2 = {};

(* build ODE system *)

Q = {{Cos[phi[t]], Sin[phi[t]]}, {-Sin[phi[t]], Cos[phi[t]]}};
d1 = {Cos[alpha1], Sin[alpha1]};
n1 = {-Sin[alpha1], Cos[alpha1]};
d2 = {Cos[alpha2], Sin[alpha2]};
n2 = {-Sin[alpha2], Cos[alpha2]};
M1 = g1'[t]*Table[d1[[i]]*n1[[j]], {i, 1, 2}, {j, 1, 2}];
M2 = g2'[t]*Table[d2[[i]]*n2[[j]], {i, 1, 2}, {j, 1, 2}];
RHS = FullSimplify[D[Q, t].Transpose[Q] + Q.(M1 + M2).Transpose[Q]];

(* solve ODE system for different angles *)

For[i = 1, i < 7, i++,
  alpha1 = Pi/4;
  alpha2 = alpha1 + Pi/2*(1 - 1/2^i);
  gammadot = 1;
  eq1 = 0 == RHS[[1, 1]];
  eq2 = gammadot == RHS[[1, 2]];
  eq3 = 0 == RHS[[2, 1]];
  tende = 2;
  s = NDSolve[{eq1, eq2, eq3, phi[0] == 0, g1[0] == 0, g2[0] == 0},
    {phi[t], g1[t], g2[t]}, {t, 0, tende} ];
  plotsphi = Append[plotsphi,
    Plot[Evaluate[phi[t] /. s], {t, 0, tende}, PlotRange -> All,
     PlotStyle -> {Black},  AxesLabel -> {"\!\(\*
StyleBox[\"t\",\nFontSlant->\"Italic\"]\)", "\[Phi]"},
     Ticks -> {Automatic,
       Table[{i*Pi/8, Row[{i, "\[Pi]/8"}]}, {i, 0, 4}]}]];
  plotsgamma1 = Append[plotsgamma1,
    Plot[Evaluate[g1[t] /. s], {t, 0, tende}, PlotRange -> All,
     PlotStyle -> {Black}, AxesLabel -> {"\!\(\*
StyleBox[\"t\",\nFontSlant->\"Italic\"]\)",
       Subscript["\[Gamma]", "1"]}]];
  plotsgamma2 = Append[plotsgamma2,
    Plot[Evaluate[g2[t] /. s], {t, 0, tende}, PlotRange -> All,
     PlotStyle -> {Black}, AxesLabel -> {"\!\(\*
StyleBox[\"t\",\nFontSlant->\"Italic\"]\)",
       Subscript["\[Gamma]", "2"]}]];
  ];

(* draw plots *)

Show[plotsphi]
Show[plotsgamma1]
Show[plotsgamma2]
```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