A Splitting Scheme for Solving Reaction-Diffusion Equations Modelling Dislocation Dynamics in Materials Subjected to Cyclic Loading

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Summary

Posing the problem

The Walgraef-Aifantis model (WA)

The numerical scheme

Results
Posing the problem

Effects of applying cyclic loads to metals and alloys:

1. Breaking the uniform spatial distribution of dislocation;
2. Raise of local strains, dislocation cells, persistent slip bands, labyrinth structures of dislocations.

The Walgraeef-Aifantis model (WA - 1985):

1. Reaction-diffusion, mesoscopic;
2. Two dislocation densities: static (dislocation forest) and mobile dislocations.
The Walgraef-Aifantis model (WA)
Ref: *J. Appl. Phys.*, **58** (1985), 668

\[
\frac{\partial \rho_s}{\partial t} = D_s \nabla^2 \rho_s + \sigma - v_s d_c \rho_s^2 - \beta \rho_s + \gamma \rho_s^2 \rho_m
\]

\[
\frac{\partial \rho_m}{\partial t} = \nabla_x \frac{1}{\gamma \rho_s^2} \nabla_x v_g \rho_m + \beta \rho_s - \gamma \rho_s^2 \rho_m
\]

where:

1. Time: measured in number of loading cycles;
2. \(\rho_s\) e \(\rho_m\): Static and mobile dislocation densities;
3. \(\sigma\): Constant rate of production of \(\rho_s\);
4. \(v_s\) e \(d_c\): Critical velocity and critical distance for the collapse of a dislocation dipole;
5. \(\beta\): Rate of conversion \(\rho_s \rightarrow \rho_m\);
6. \(\gamma\): Rate of capture of mobile dislocations by a dipole;
Solving the WA model

1. Finite differences, second order in time, rectangular domain;
2. The target scheme - nonlinear
3. Achieving second order: internal iterations at each time step;
4. Decoupling rows and columns: splitting scheme (Stabilizing correction).
The target scheme

\[
\begin{align*}
\frac{\rho_{s}^{n+1} - \rho_{s}^{n}}{\Delta t} &= \Lambda_{x}^{n+1/2} \frac{\rho_{s}^{n+1} + \rho_{s}^{n}}{2} + \Lambda_{y}^{n+1/2} \frac{\rho_{s}^{n+1} + \rho_{s}^{n}}{2} + f_{1}^{n+1/2} \\
\frac{\rho_{m}^{n+1} - \rho_{m}^{n}}{\Delta t} &= \Lambda_{2}^{n+1/2} \frac{\rho_{m}^{n+1} + \rho_{m}^{n}}{2} + f_{2}^{n+1/2}
\end{align*}
\]

Main features:

1. Nonlinear, with two coupled equations;
2. Algebraic equations of lines coupled to the equations of columns: high computational cost;
3. The factor 2 is included in the definition of operators \(\Lambda_{x}^{n+1/2}\), \(\Lambda_{y}^{n+1/2}\) and \(\Lambda_{2}^{n+1/2}\).
Internal iterations

\[
\frac{\rho_{s}^{n+1,k+1} - \rho_{s}^{n}}{\Delta t} = \left( \Lambda_{x}^{n+1/2,k} + \Lambda_{y}^{n+1/2,k} \right) \frac{\rho_{s}^{n+1,k+1}}{2} + \rho_{s}^{n} + f_{1}^{n+1/2,k}
\]

\[
\frac{\rho_{m}^{n+1,k+1} - \rho_{m}^{n}}{\Delta t} = \Lambda_{2}^{n+1/2,k} \frac{\rho_{m}^{n+1,k+1}}{2} + \rho_{m}^{n} + f_{2}^{n+1/2,k}
\]
Definition of operators – first equation

\[ \frac{\partial \rho_s}{\partial t} = D_s \nabla^2 \rho_s + \sigma - v_s d_c \rho_s^2 - \beta \rho_s + \gamma \rho_s^2 \rho_m \]

\[ \frac{\rho^{n+1,k+1}_s - \rho^n_s}{\Delta t} = \Lambda^{n+1/2,k}_x \rho_s^{n+1,k+1} + \rho^n_s + \frac{1}{2} \Lambda^{n+1/2,k}_y \rho_s^{n+1,k+1} + \rho^n_s + f_1^{n+1/2} \]

\[ \Lambda^{n+1/2,k}_x = \frac{D_s}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{4} v_s d_c \left( \frac{\rho_s^{n+1,k} + \rho^n_s}{2} \right) - \frac{\beta}{4} \]

\[ \Lambda^{n+1/2,k}_y = \frac{D_s}{2} \frac{\partial^2}{\partial y^2} - \frac{1}{4} v_s d_c \left( \frac{\rho_s^{n+1,k} + \rho^n_s}{2} \right) - \frac{\beta}{4} \]

\[ f_1^{n+1/2,k} = \sigma + \frac{\gamma}{2} \left( \frac{\rho_s^{n+1,k} + \rho^n_s}{2} \right)^2 \left( \rho_m^{n+1,k} + \rho^n_m \right) - \frac{\beta}{2} \rho^n_s \]
Definition of operators – second equation

\[ \frac{\partial \rho_m}{\partial t} = \nabla_x \frac{v_g}{\gamma \rho_s^2} \nabla_x v_g \rho_m + \beta \rho_s - \gamma \rho_s^2 \rho_m \]

\[ \frac{\rho_{m}^{n+1,k+1} - \rho_{m}^{n}}{\Delta t} = \Lambda_{2}^{n+1/2} \frac{\rho_{m}^{n+1,k+1}}{2} + \rho_{m}^{n} + f_{2}^{n+1/2} \]

\[ \Lambda_{2}^{n+1/2,k} = \frac{1}{2} \frac{\partial}{\partial x} \frac{1}{\gamma \left( \frac{\rho_s^{n+1,k} + \rho_s^n}{2} \right)} \frac{\partial}{\partial x} v_g - \gamma \left( \frac{\rho_s^{n+1,k} + \rho_s^n}{2} \right)^2 \]

\[ f_{2}^{n+1/2,k} = \beta \left( \frac{\rho_s^{n+1,k} + \rho_s^n}{2} \right) \]
The alternative scheme

The target scheme is replaced by an alternative one, featuring:

1. Iterative (linear), semi-implicit;
2. Stabilizing terms: implicit;
3. Destabilizing terms: explicit;
4. First equation \(\rightarrow\) replaced by two others \((splitting)\), to save memory and avoid large linear systems;
Splitting of the first equation

The original scheme of the first equation

\[
\frac{\rho_{s}^{n+1,k+1} - \rho_{s}^{n}}{\Delta t} = \left( \Lambda_{x}^{n+1/2,k} + \Lambda_{y}^{n+1/2,k} \right) \frac{\rho_{s}^{n+1,k+1}}{2} + \rho_{s}^{n} + f_{1}^{n+1/2,k}
\]

The equivalent scheme:

\[
\frac{\tilde{\rho}_{s} - \rho_{s}^{n}}{\Delta t} = \Lambda_{x}^{n+1/2,k} \tilde{\rho}_{s} + 2\Lambda_{y}^{n+1/2,k} \rho_{s}^{n} + \Lambda_{x}^{n+1/2} \rho_{s}^{n} + f_{1}^{n+1/2}
\]

\[
\frac{\rho_{s}^{n+1,k+1} - \tilde{\rho}_{s}}{\Delta t} = \Lambda_{y}^{n+1/2,k} \left( \rho_{s}^{n+1,k+1} - \rho_{s}^{n} \right)
\]

Main features of the scheme:

- Error of same order of the original;
- More stable than the original;
- Does not change the steady state solution.
Splitting of the first equation

The original scheme:

\[
\frac{\rho_{s}^{n+1,k+1} - \rho_{s}^{n}}{\Delta t} = \left( \Lambda_{x}^{n+1/2,k} + \Lambda_{y}^{n+1/2,k} \right) \frac{\rho_{s}^{n+1,k+1} + \rho_{s}^{n}}{2} + f_{1}^{n+1/2,k}
\]

The equivalent scheme:

\[
\left( I + \Delta t^2 \Lambda_{x}^{n+1/2i,k} \Lambda_{y}^{n+1/2,k} \right) \frac{\rho_{s}^{n+1,k+1} - \rho_{s}^{n}}{\Delta t} = \left( \Lambda_{x}^{n+1/2,k} + \Lambda_{y}^{n+1/2,k} \right) \frac{\rho_{s}^{n+1,k+1} + \rho_{s}^{n}}{2} + f_{1}^{n+1/2,k}
\]

The scheme is equivalent to the original one, except for the positive operator with norm $> 1$:

\[
B \equiv I + \Delta t^2 \Lambda_{x}^{n+1/2,k} \Lambda_{y}^{n+1/2,k} = I + \mathcal{O} \left( \Delta t^2 \right)
\]
Results - linear diffusion of $\rho_s$

Time evolution of $\rho_s$

$t = 0.75$

$t = 1.50$

$t = 1.70$

$t = 1.80$

$t = 1.82$

$t = 2.00$

$t = 3.00$

$t = 12.0$
Results - linear diffusion of $\rho_s$

Time evolution of $\rho_s$ – linear diffusion

$t = 50.0$

$t = 70.0$

$t = 150.0$

$t = 700.0$

$t = 1000.0$

$t = 1500.0$

$t = 2000.0$

$t = 2524.0$
Results - linear diffusion of $\rho_s$

Rate of change of the distance between two successive states $\times t$

$$L_1 = \frac{1}{\Delta t} \frac{\sum_{ij} |\rho_{s}^{n+1} - \rho_{s}^{n}| + \sum_{ij} |\rho_{m}^{n+1} - \rho_{m}^{n}|}{\sum_{ij} |\rho_{s}^{n+1}| + \sum_{ij} |\rho_{m}^{n+1}|}$$
Results - nonlinear diffusion of $\rho_s$

Time evolution of $\rho_s$ – nonlinear diffusion

- $\beta = 15$, $t = 0, 50$
- $\beta = 30$, $t = 1, 00$
- $\beta = 60$, $t = 0, 50$
- $\beta = 15$, $t = 7, 0$
- $\beta = 30$, $t = 20, 0$
- $\beta = 60$, $t = 8, 00$
- $\beta = 15$, $t = 150, 0$
- $\beta = 30$, $t = 572, 0$
- $\beta = 60$, $t = 300, 0$
- $\beta = 15$, $t = 1748, 0$
- $\beta = 30$, $t = 5648, 0$
- $\beta = 60$, $t = 2395, 0$
Results - nonlinear diffusion of $\rho_s$
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