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Central South University
相图、相变、材料设计与制备科学中心
Science Center for Phase Diagram, Phase Transtion, Materials Design and Preparation
硬质合金微结构研究小组
"Microstructure in Cemented Carbide" Cooperation Group
中德"微结构"联合实验室
Sino-German Cooperation Group "Microstructure"

多物理场耦合的 **相场模拟软件（MInDeS）** 开发

——固体力学模块

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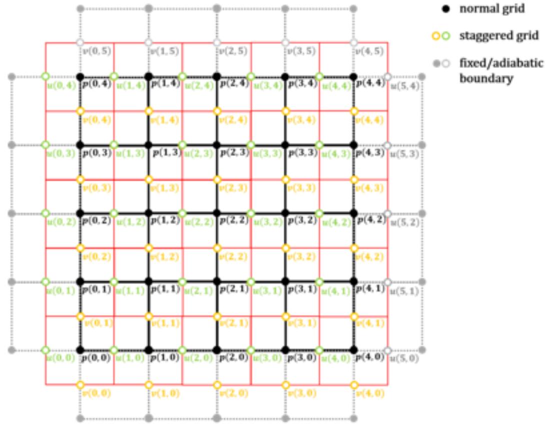
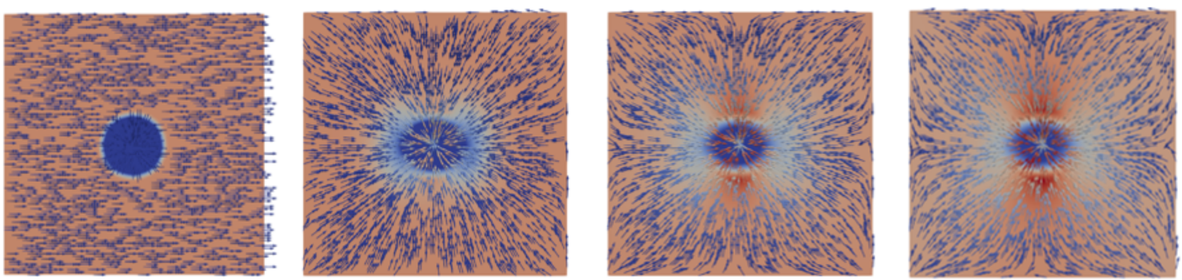
1、机械平衡求解

1.1 显式差分法

- $\sigma = C:(\epsilon - \epsilon^{*})$　　应力求解
- $\rho \dfrac{\partial^2 \boldsymbol{u}}{\partial t^2} = \nabla \cdot \sigma$　　动量平衡
- $\epsilon_{ij} = \dfrac{1}{2}\left(\dfrac{\partial u_i}{\partial r_j} + \dfrac{\partial u_j}{\partial r_i}\right) + \varepsilon_{ij}^{app}$ 小应变模型
- **位移场迭代至机械平衡：**





1、机械平衡求解

1.2 半隐式光谱法

- 半隐式求解位移场

$$\frac{\partial u_i(\vec{r})}{\partial r_j} = \int_{|\vec{k}\neq 0|} \left\{ n_j \Omega_{ij}(\vec{n}) \int_V \left[C_{ijkl}(\vec{r})\varepsilon^*_{kl}(\vec{r}) + \left(C^0_{ijkl} - C_{ijkl}(\vec{r}) \right) \varepsilon_{kl}(\vec{r}) \right] e^{-i\vec{k}\vec{r}} d^3r \right\} e^{i\vec{k}\vec{r}} \frac{d^3k}{(2\pi)^3}$$

- 边界条件求解

> 求模拟域平均应力： $\bar{\sigma}_{ij} = \frac{1}{V}\int_V \left\{ C_{ijkl}(\vec{r}) \left[\frac{1}{2}\left(\frac{\partial u_i(\vec{r})}{\partial r_j} + \frac{\partial u_j(\vec{r})}{\partial r_i} \right) - \varepsilon^*_{kl}(\vec{r}) \right] \right\} d^3r$

> 根据外加应力求对应的外加应变： $\sigma^{tag}_{ij} = \sigma^{app}_{ij} - \bar{\sigma}_{ij}$ ， $\varepsilon^{app}_{ij} = S_{ijkl}(\vec{r})\sigma^{tag}_{ij}$

> 若设定的为外加应变，将直接设置外加应变： ε^{app}_{ij}

- 小应变模型求总应变

$$\varepsilon_{ij}(\vec{r}) = \frac{1}{2}\left(\frac{\partial u_i(\vec{r})}{\partial r_j} + \frac{\partial u_j(\vec{r})}{\partial r_i} \right) + \varepsilon^{app}_{ij}$$

- 迭代求解位移场、应力场及应变场，得机械平衡。

2、塑性屈服求解

2.1 屈服准则：Prandtl–Reuss 模型

$$f\left((\sigma^{el})', \bar{\epsilon}^{pl}\right) := \left\|(\sigma^{el})'\right\| - \sqrt{\frac{2}{3}}\left(f_y(\phi) + H(\phi)\bar{\epsilon}^{pl}\right) \leq 0$$

- $(\sigma^{el})' = \sigma^{el} - \frac{1}{3}\left(\sigma_{11}^{el} + \sigma_{22}^{el} + \sigma_{33}^{el}\right)\mathbf{1}$
- $f_y(\phi) = \sum_\alpha f_y^\alpha h(\phi^\alpha)$ $\qquad H(\phi) = \sum_\alpha H^\alpha h(\phi^\alpha)$
- **求解法：**
- 纯弹性预测(t^{n+1})：$\left(\sigma^{trial}\right)^{n+1} = C:\left((\epsilon)^{n+1} - \left(\epsilon^{pl}\right)^n\right)$
- 屈服检测：若$f\left[\left(\sigma^{trial}\right)'^{n+1}, \left(\bar{\epsilon}^{pl}\right)^n\right] > 0$，则进行塑性求解：
  - 计算塑性求解量级$(\Delta\gamma)$：$\Delta\gamma = \dfrac{f\left[\left(\sigma^{trial}\right)'^{n+1}, \left(\bar{\epsilon}^{pl}\right)^n\right]}{2\mu(\phi) + \frac{2}{3}H(\phi)}$
  - $\left(\bar{\epsilon}^{pl}\right)^{n+1} = \left(\bar{\epsilon}^{pl}\right)^n + \sqrt{\frac{2}{3}}\Delta\gamma$
  - $\left(\epsilon^{pl}\right)^{n+1} = \left(\epsilon^{pl}\right)^n + \Delta\gamma \dfrac{\left(\sigma^{trial}\right)'^{n+1}}{\left\|\left(\sigma^{trial}\right)'^{n+1}\right\|}$
  - $\left(\sigma^{trial}\right)'^{n+1} = \left(\sigma^{trial}\right)'^{n+1} - 2\mu(\phi)\Delta\gamma \dfrac{\left(\sigma^{trial}\right)'^{n+1}}{\left\|\left(\sigma^{trial}\right)'^{n+1}\right\|}$
  - $\mu(\phi) = \sum_\alpha \mu^\alpha h(\phi^\alpha)$

迭代至 $f\left[\left(\sigma^{trial}\right)'^{n+1}, \left(\bar{\epsilon}^{pl}\right)^n\right] < 0$

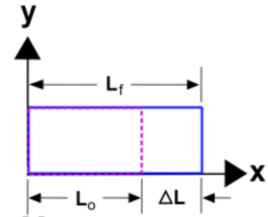
3、应变模型

3.1 小应变模型

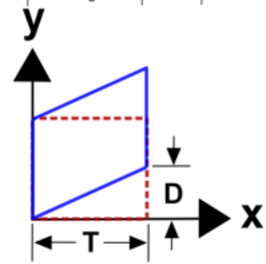
- 当形变量微小，忽略形变对质点空间位置的影响，在参考构型上计算位移梯度：

$$
\begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{bmatrix} = \epsilon = \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{yz} \\ \epsilon_{xz} \\ \epsilon_{xy} \end{bmatrix} = \begin{bmatrix} \dfrac{\partial u_x}{\partial r_x} \\ \dfrac{\partial u_y}{\partial r_y} \\ \dfrac{\partial u_z}{\partial r_z} \\ \dfrac{1}{2}\left(\dfrac{\partial u_y}{\partial r_z} + \dfrac{\partial u_z}{\partial r_y}\right) \\ \dfrac{1}{2}\left(\dfrac{\partial u_x}{\partial r_z} + \dfrac{\partial u_z}{\partial r_x}\right) \\ \dfrac{1}{2}\left(\dfrac{\partial u_x}{\partial r_y} + \dfrac{\partial u_y}{\partial r_x}\right) \end{bmatrix}
$$

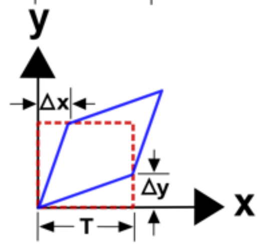
$$\epsilon = \frac{\Delta L}{L_0}$$



$$\gamma = \frac{D}{T}$$



$$\gamma = \frac{\Delta x + \Delta y}{T}$$

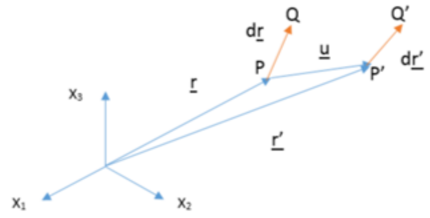


3、应变模型

3.2 有限应变模型 （暂未实现）

- 当空间微小元PQ因形变变成P'Q'，形变量不可忽略，在当前构型上计算位移梯度：

… …

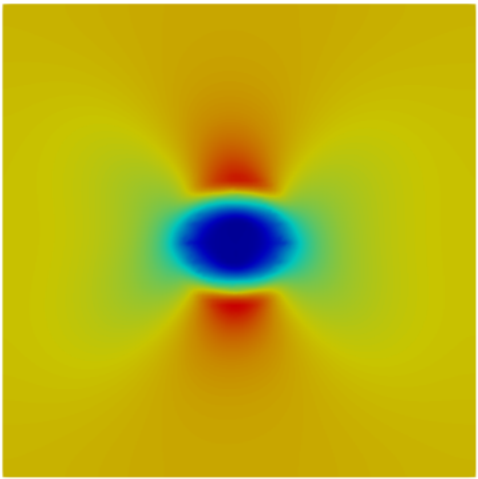


4、模型测试

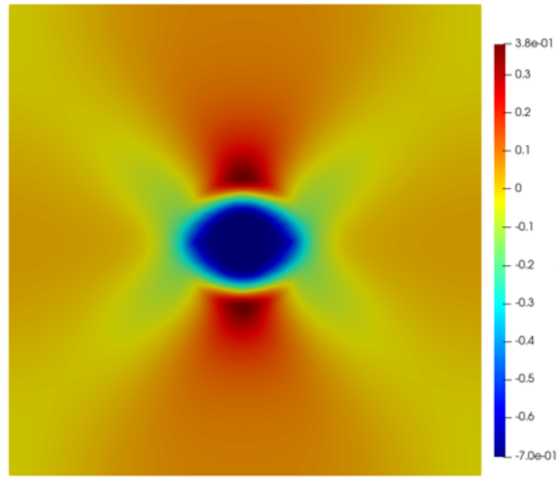
4.1 纯弹性 - 显式差分法、半隐式光谱法对比

- 2维 - 颗粒夹杂:

显式



隐式



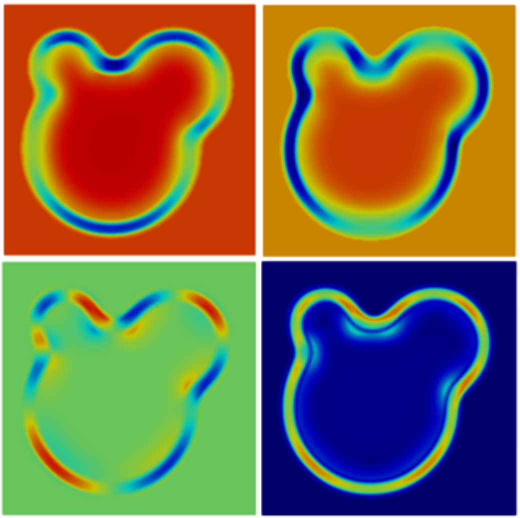
	显式	隐式
求解步数:	8548	5
应变精度:	1e-6	1e-6
耗时(s)　:	75.795	0.211

4、模型测试

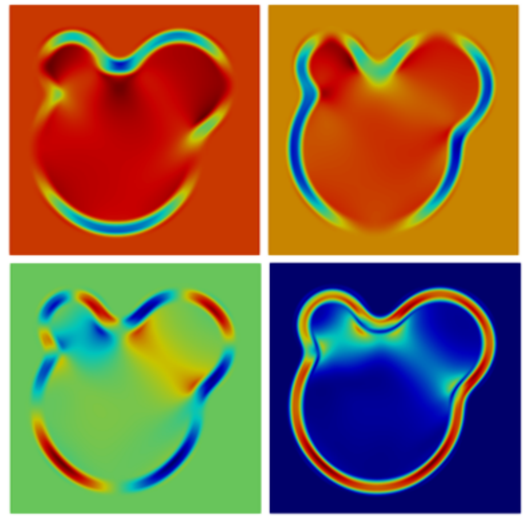
4.1 纯弹性 - 显式差分法、半隐式光谱法对比

- 2维 – 复杂形貌、不均匀弹性模量、本征应变：

显式



隐式

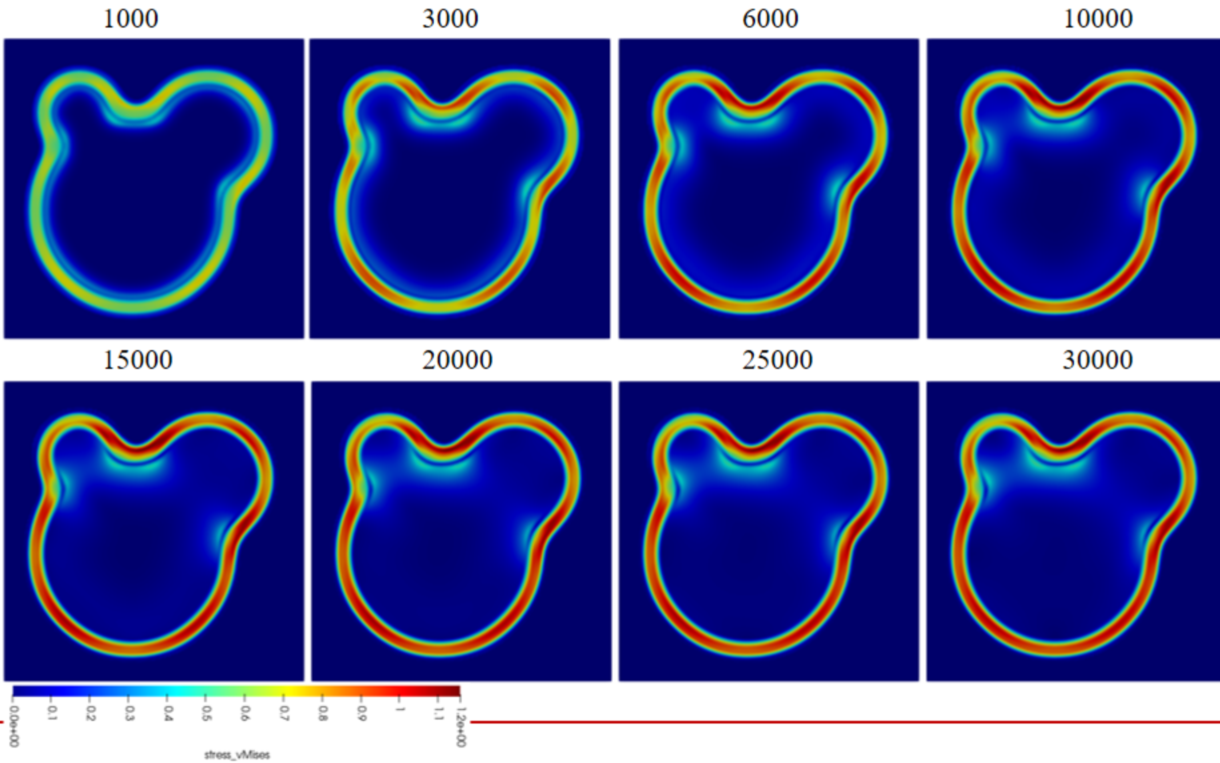


	显式	隐式
求解步数:	3783	21
应变精度:	1e-5	1e-4 (1e-5 收敛失败)
耗时(s) :	132.833	1.377

4、模型测试

4.1 纯弹性 - 显式差分法、半隐式光谱法对比

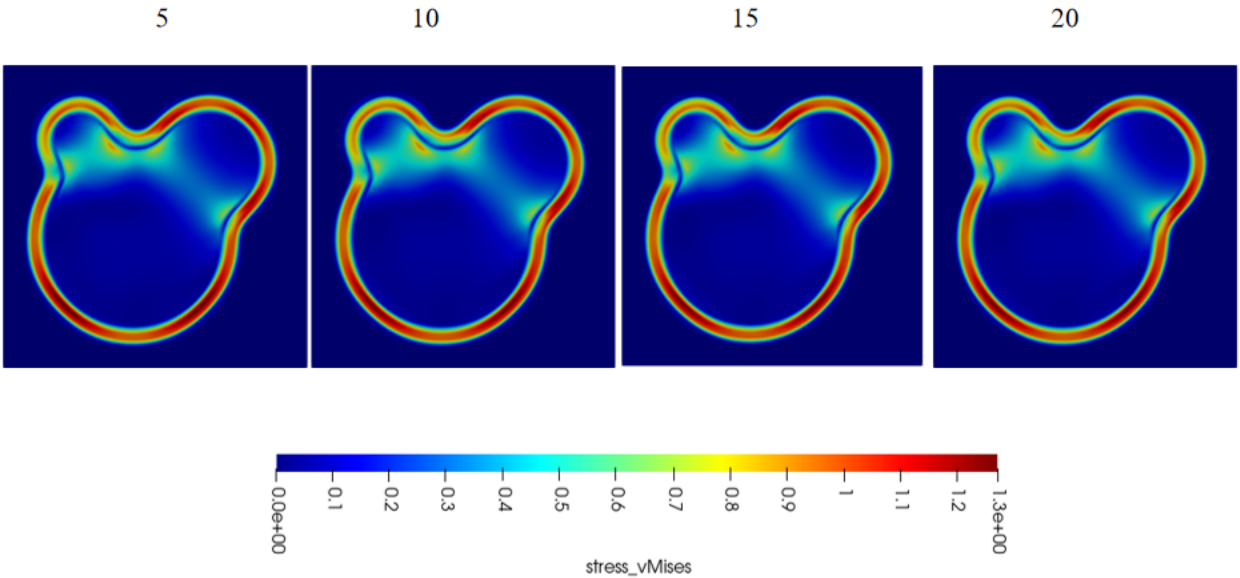
- 收敛步数的影响 - 显式



4、模型测试

4.1 纯弹性 - 显式差分法、半隐式光谱法对比

- 收敛步数的影响 – 隐式



4、模型测试

4.2 半隐式机械平衡求解 + 塑性求解

- **研究对象，铁素体内的纯弹性夹杂物**
- 铁素体（m）：$E_m = 210\text{Gpa}, v_m = 0.288, f_{y_m} = 275\text{Mpa}, H_m = 0.1\text{Mpa}$
- 夹杂物（i）：$E_i = 10\text{Gpa}, \quad v_i = 0.288, \quad f_{y_i} = 10^3 f_{y_m}, \quad H_i = 10H_m$

- **二维结构：**

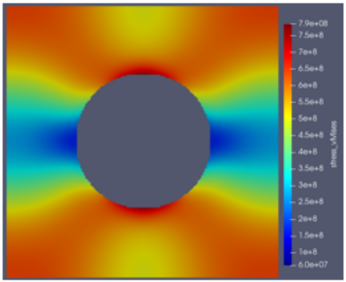
X 方向施加动态应变

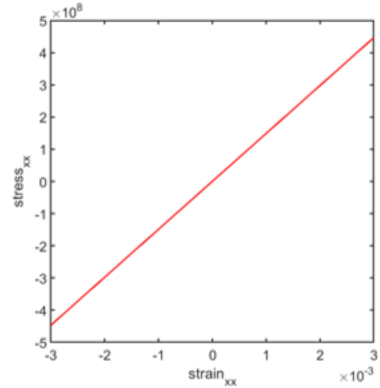
Small strain elasto-plastic multiphase-field model, Daniel Schneider, Stefan Schmid, Michael Selzer, Thomas Böhlke, Britta Nestler

4、模型测试

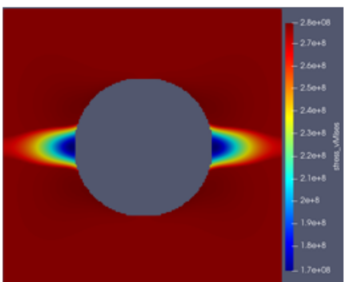
4.2 半隐式机械平衡求解 + 塑性求解

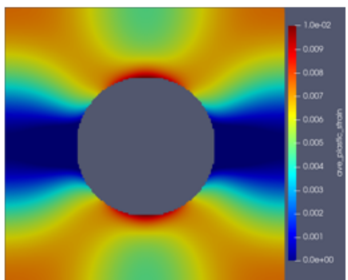
- 研究对象，铁素体内的纯弹性夹杂物
- Pure elasticity:

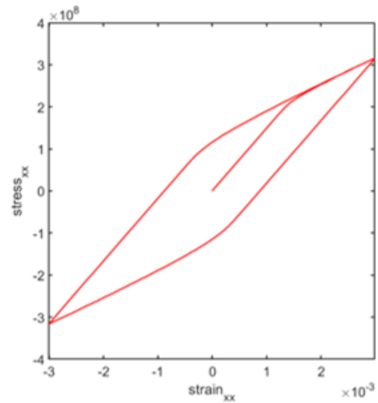




- Elasticity + plasticity







4、模型测试

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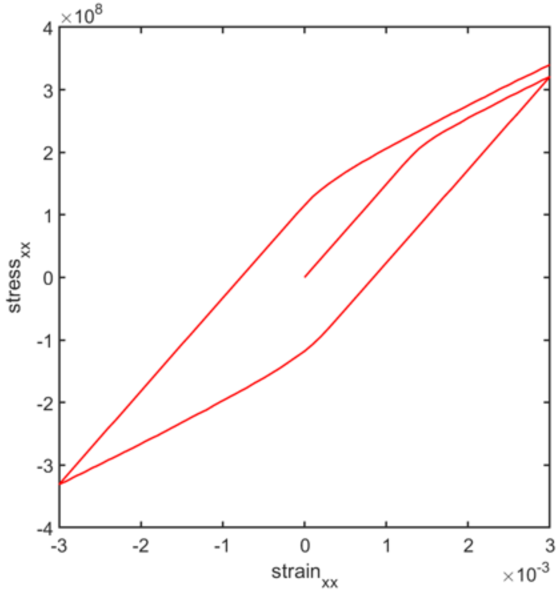
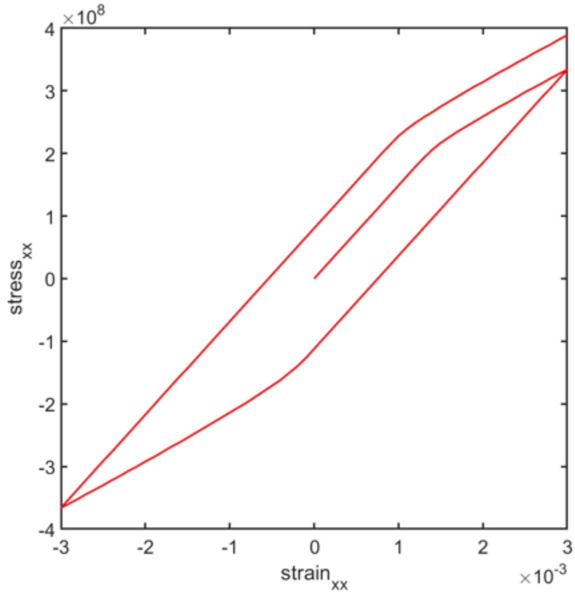
- 夹杂物（i）：$E_i = 10\text{Gpa},\ \ v_i = 0.288,\ \ f_{y_i} = 10^3 f_{y_m},\ \ H_i = 10H_m$

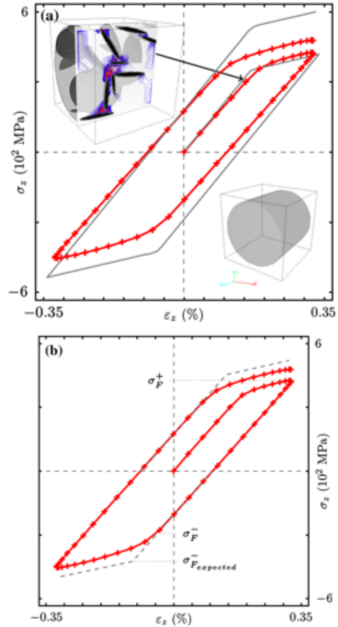


4、模型测试

4.2 半隐式机械平衡求解 + 塑性求解

- **研究对象，铁素体内的纯弹性夹杂物**
- 铁素体（m）：$E_m = 210\text{Gpa}, v_m = 0.288, f_{y_m} = 275\text{Mpa}, H_m = 40\text{Gpa}$
- 夹杂物（i）：$E_i = 10\text{Gpa},\ \ v_i = 0.288,\ \ f_{y_i} = 10^3 f_{y_m},\ \ H_i = 10H_m$
- 时间：57.938 s



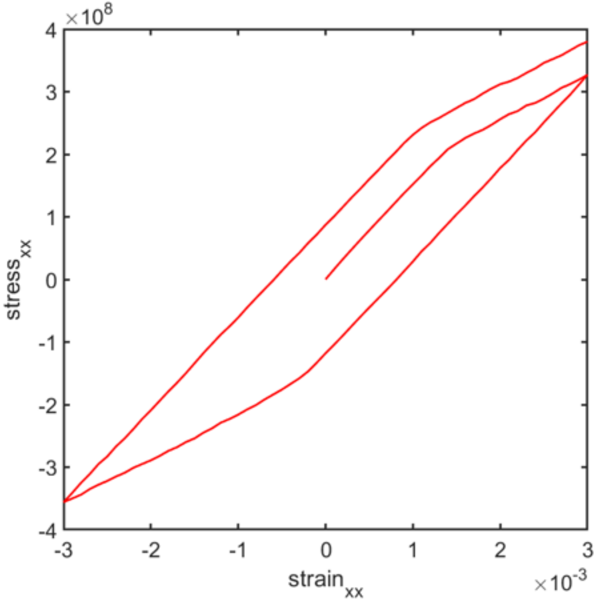


Small strain elasto-plastic multiphase-field model, Daniel Schneider, Stefan Schmid, Michael Selzer, Thomas Böhlke, Britta Nestler

4、模型测试

4.3 显式机械平衡求解 + 塑性求解

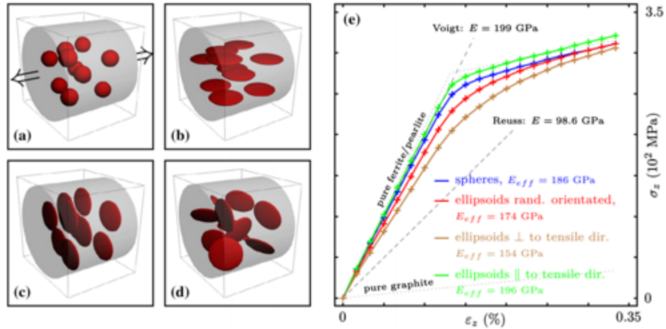
- **研究对象，铁素体内的纯弹性夹杂物**
- 铁素体（m）：$E_m = 210\text{Gpa}, v_m = 0.288, f_{y_m} = 275\text{Mpa}, H_m = 40\text{Gpa}$
- 夹杂物（i）：$E_i = 10\text{Gpa}, \quad v_i = 0.288, \quad f_{y_i} = 10^3 f_{y_m}, \quad H_i = 10H_m$
- 时间：3.255 小时



5、应用展望

5.1 应用案例

- 夹杂物对材料体力学性能的影响



- 脆性、韧性 或 复合材料裂纹