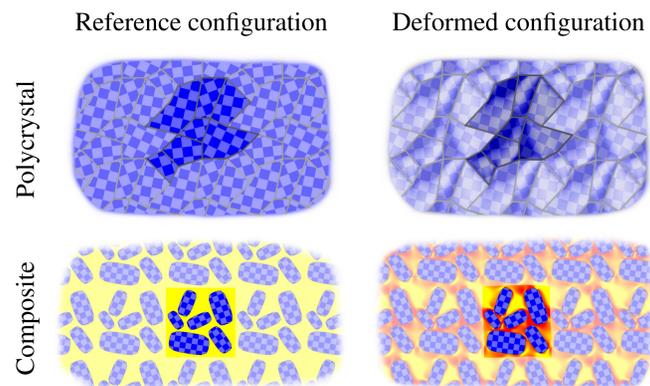


## 1 INTRODUCTION

Ferromagnetic shape-memory materials exhibit comparably large strains in response to an applied magnetic field. For single crystals one can achieve strains of order of magnitude 10%. Single crystals are problematic both productionwise and due to their brittleness.

In the search for applicable devices, polycrystal samples have been explored. In polycrystals the effectivity drops significantly, as a consequence of the rigidity of interacting non-aligned grains. Here we investigate the role of misalignment numerically and quantify its impact on the effective spontaneous strain.

A recently-proposed alternative for shape memory devices is to embed small single-crystal shape-memory particles in a soft polymer matrix. This approach gives a large freedom in the material development. We exemplarily demonstrate the potential of this approach and show that a significant percentage of the single-crystal spontaneous strain can be realized in polymer composites.



The figure shows a finite portion of two periodic samples, containing grains or particles with different orientations. The checkerboard pattern illustrates the lattice orientation, the shading the elastic energy density.

## 2 MICROMAGNETIC-ELASTIC MODEL

We work on a domain  $\Omega \subset \mathbb{R}^2$  occupied by a polycrystal, which consists of grains  $\omega_i$ , each of which is a single crystal. In the case of polymer composites, the  $\omega_i$  denote the particles in a polymer matrix  $\Omega \setminus \omega$ . In both cases,  $\omega = \cup \omega_i$ .

**Kinematics.** Let  $u : \Omega \rightarrow \mathbb{R}^2$  be the elastic displacement. We assume the elastic deformation  $v(x) = x + u(x)$  to be injective on  $\Omega$ , and use linear elasticity throughout. Let  $p : \omega \rightarrow \{1, 2\}$  be the phase index, which is supposed to be constant on each grain (each particle), and  $M : \mathbb{R}^2 \rightarrow \mathbb{R}^2$  the magnetization.

**Elasticity.** The particles have two energy-minimizing phases, distinguished by the phase parameter  $p$ . Their elastic energy is

$$E_{\text{elast}}^{\text{MSM}} = \int_{\omega} W^{\text{MSM}}((\nabla v(x))Q(x) - \varepsilon_{p(x)}) dx.$$

Here  $Q : \omega \rightarrow SO(2)$  represents the crystal lattice orientation in the reference configuration,  $\varepsilon_p$  is the eigenstrain of phase  $p$ ,

$$\varepsilon_1 = \begin{pmatrix} -\varepsilon_0 & 0 \\ 0 & \varepsilon_0 \end{pmatrix}, \quad \varepsilon_2 = \begin{pmatrix} \varepsilon_0 & 0 \\ 0 & -\varepsilon_0 \end{pmatrix},$$

and  $W^{\text{MSM}}(F)$  is a cubic elastic energy, parameterized by  $C_{11}$ ,  $C_{12}$  and  $C_{44}$ .

In composites we additionally have the elastic energy of the polymer matrix, which is assumed to be an isotropic, linearly elastic material:

$$E_{\text{elast}}^{\text{polymer}} = \int_{\Omega \setminus \omega} W^{\text{polymer}}(v(x)) dx.$$

**Micromagnetism.** Let  $M = M_s m$  be the magnetization. Here  $M_s$  is the saturation magnetization, and  $m : \mathbb{R}^2 \rightarrow \mathbb{R}^2$  has unit length on the deformed domain  $v(\omega)$ , i.e., on the grains (particles), and vanishes elsewhere. The magnetic energy is given by the coupling to the external field  $H_{\text{ext}}$ , the demagnetization term, and the phase-dependent anisotropy term:

$$\begin{aligned} E_{\text{demag}} &= \frac{1}{2} \frac{M_s^2}{\mu_0} \int_{\mathbb{R}^2} |H_d|^2 dy, \\ E_{\text{ext}} &= -\frac{M_s}{\mu_0} \int_{\mathbb{R}^2} H_{\text{ext}} \cdot m dy, \\ E_{\text{aniso}} &= K_u \int_{v(\omega)} \varphi_{p(v^{-1}(y))} ((R_{\nabla v \circ v^{-1}} Q(y))^T m) dy. \end{aligned}$$

The field  $H_d : \mathbb{R}^2 \rightarrow \mathbb{R}^2$  is the projection of  $m$  onto curl-free fields. Furthermore,  $\varphi_2(m) = \frac{m_1^2}{|m|^2}$ ,  $\varphi_1(m) = \frac{m_2^2}{|m|^2}$  are the two magnetic anisotropy functions reflecting the phase-dependent easy axis, and  $K_u$  is the uniaxial anisotropy constant. The matrix  $R_{\nabla v(x)} \in SO(2)$  is the rotation associated with the elastic deformation  $v$  at a reference point  $x$ ,  $R \approx \text{Id} + \frac{1}{2}(\nabla v - (\nabla v)^T)$ .

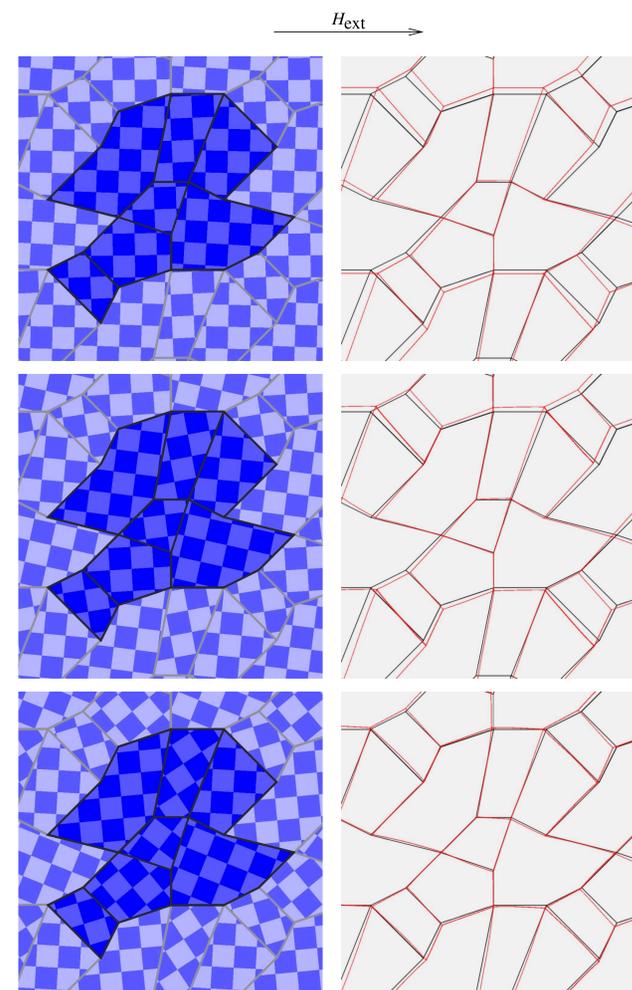
**Homogenization and numerical methods.** In the spirit of the theory of homogenization, we study periodic configurations, where each periodic cell contains a small number of particles. We use boundary elements to express both the elastic and the magnetic problem in the full space in terms of the deformation and the magnetization on the boundary of each grain (particle).

**Material parameters.** We use parameters for NiMnGa, precisely:  $\frac{M_s}{\mu_0} \simeq 0.50 \frac{\text{MPa}}{\text{T}}$ ,  $K_u \simeq 0.13 \text{ MPa}$ ,  $\varepsilon_0 \sim 0.058$ ,  $C_{11} = 160 \text{ GPa}$ ,  $C_{44} = 40 \text{ GPa}$ ,  $C_{11} - C_{12} = 4 \text{ GPa}$ . For the polymer we take  $\lambda \sim 20 \text{ GPa}$ ,  $\mu \sim 1 \text{ GPa}$ .

## 3 POLYCRYSTALS

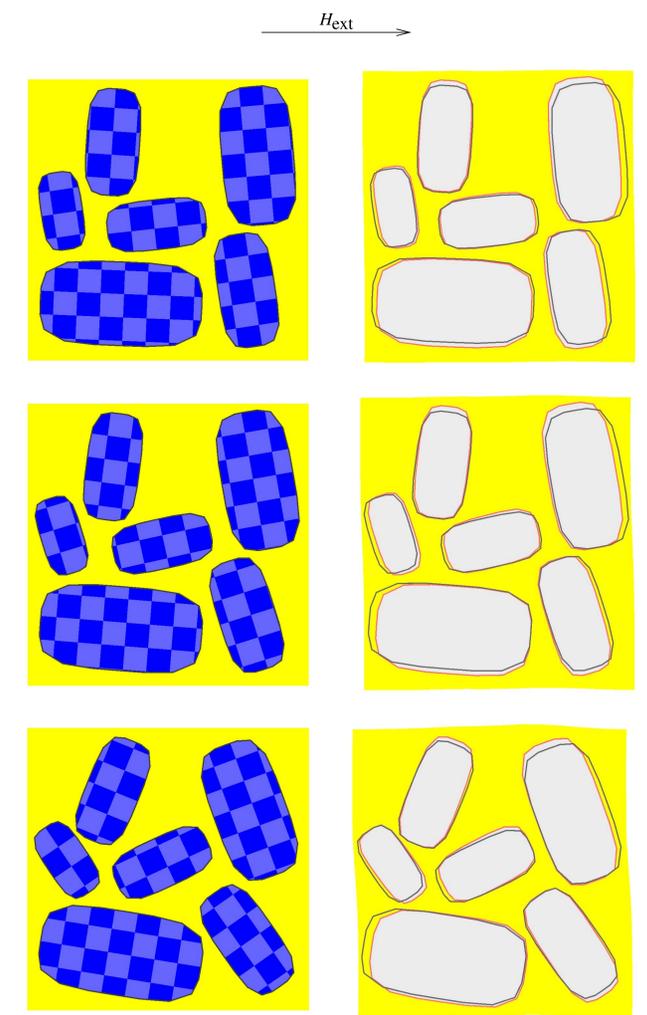
We investigate magnetostriction in a periodic polycrystal. For better comparison, we keep the grain geometry (i.e. the  $\omega_i$ ) fixed, and vary only the lattice orientation in the grains (i.e. the  $Q_i$ ). We show results for three different choices of the orientation, ranging from almost oriented to completely random. The first column shows the reference configuration, the second one the deformed state at the spontaneous deformation, with an applied horizontal external field  $H_{\text{ext}} = 1T$ .

Average mismatch	Spontaneous strain	Relative strain
2°	5.6%	96%
8°	4.2%	72%
22.5° (random)	1.6%	27%
0 (single crystal)	5.8%	100%



## 4 COMPOSITES

As a second case we consider polymer composites. Again, we keep the shape and size (total volume fraction 50%) of the particles fixed, and vary their orientation. The dependence of the macroscopic magnetostriction on the orientation is much smaller than for polycrystals. In particular, misorientations of 2° (first line) and 8° (second line) give almost exactly the same result, which in turn is comparable to the one of the polycrystal at 8° misorientation. Even in the non-oriented case (third line) the composite recovers almost one-half of the single-crystal magnetostriction. The spontaneous strain is 3.7%, 3.9% and 2.9% in the three cases, compared to the 5.8% in case of a single crystal.



## REFERENCES

- [1] CONTI, S., LENZ, M., AND RUMPF, M. Modeling and simulation of magnetic shape-memory polymer composites. preprint, 2006.