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MODELLING OF COMPLEX ELASTIC CRYSTALS BY MEANS OF MICROMORPHIC GYROCONTINUA

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Summary We model elastic crystals with a complex deformable unit cell containing many gyroscopic subparticles. To obtain the equations of this medium we use two approaches, phenomenological and microstructural. The phenomenological approach is based on the fundamental laws of balance of mechanics. We introduce analogues for the stress and the couple tensor for this micromorphic gyroscopic continuum. For the microstructural consideration we model the interaction between subparticles as a potential interaction of general kind between rigid bodies both of force and torque nature. We sum the laws of the balance of linear and angular momentum over all subparticles of a cell. To pass from the discrete model to the continuum we expand these laws in space co-ordinates of different scale; one scale is concerned with the distance between subparticles, and another with the cell size. This theory may have applications for the description of magnetic crystals.

INTRODUCTION

The most interesting crystals from the point of view of magnetoacoustic interaction are ferrite crystals with a complicated structure, such as Yttrium-Iron Garnets (YIG). Each cell of such a crystal consists of many atoms, combined in clusters. Atoms of Fe are responsible for magnetic properties of the crystal. They interact with each other in a complicated way via the neighbouring atoms of oxygen and yttrium. The total number of atoms in the cell is more than 100. The interaction between neighbouring clusters is essential, but not the interaction between the clusters of the same cell if they are not neighbours. The magnetic moment of clusters is related to the angular momentum (including moment of momentum and spin). A cell contains several clusters possessing spin, and it is deformable. We suggest as an approximation to model such a cell as a deformable particle containing several interacting subparticles – infinitesimal rigid bodies possessing spin.

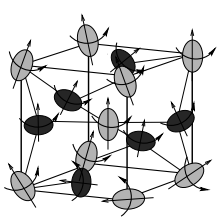

Figure 1. 1/8 of a cell of the Yttrium-Iron Garnet. Distribution of Fe.

PHENOMENOLOGICAL APPROACH

Let us first consider the medium as an inhomogeneous elastic Kelvin medium ([1]): each cluster corresponds to a point-body, which is an infinitesimal rigid point-body, able to perform rotations and translations of a general kind, and possessing rotational symmetry. Point-bodies interact with their neighbours. Suppose this interaction to be determined only by the geometrical configuration at the given moment in time. The rotations of a point-body around its axis do not induce stresses in the medium. In each point we write down the laws of balance of force and torque in Piola form:

$$\overset{\circ}{\nabla}\cdot\mathbf{T}+\rho_0\,\mathbf{Q}=\rho_0\,\ddot{\mathbf{u}},\qquad \overset{\circ}{\nabla}\cdot\mathbf{M}+(\mathbf{G}^{\top}\cdot\mathbf{T})_{\times}+\rho_0\,\mathbf{C}=\rho_0\,(\boldsymbol{\Theta}\cdot\boldsymbol{\omega})^{\cdot}, \tag{1}$$

where $\mathbf{T},\mathbf{M}$ are the first Piola-Kirchoff stress and couple stress tensors, $\mathbf{G}$ is the gradient of radius-vector, $\mathbf{Q},\mathbf{C}$ are external body force and torque, and in the right side of equations we have the inertial terms. We have two scales in space, one ("macro-scale") corresponds to the size of the cell, and another one ("micro-scale") to the distance between a point-body and its neighbours. The gradient $\overset{\circ}{\nabla}$ is the gradient in "micro-co-ordinates" in the reference configuration. The constitutive equations for this medium may be obtained from the law of balance of energy and objectivity requirements [1], so the system (1) is closed.

We pass to the homogeneous continuum, integrating over the initial volume V_0 of the cell equations (1), supposing that all the quantities are sufficiently smooth in the "macro-co-ordinates". Now a "point-body" of the medium is not any more a gyroscopic subparticle, but the cell itself. We obtain "macro"-analogues for the first Piola-Kirchhoff stress and couple stress tensors:

$$\partial_{\mathbf{s}}\cdot\overline{\mathbf{T}}+\frac{1}{V_0}\int_{V_0}\rho_0\mathbf{K}\,dV_0=\rho_0\ddot{\mathbf{S}}, \tag{2}$$

where $\partial_{\mathbf{s}}$ is the "macro-gradient" in the reference configuration, $\mathbf{S}$ is the centre of mass of the cell ("macro-co-ordinate"), $\overline{\mathbf{T}} = \mathbf{a}_i\mathbf{n}^i \cdot \frac{1}{V_0}\int_{\Sigma_{-i}} \mathbf{T}\, d\Sigma_{-i}$ is the "first Piola-Kirchhoff macro-stress tensor", $\mathbf{a}_i$ is a basic vector of the lattice, $\mathbf{n}^i$ is the normal to the surface of the cell Σ_i, and

$$\partial_{\mathbf{s}} \cdot \overline{\mathbf{M}} + [\partial_{\mathbf{s}}\mathbf{S}^\top \cdot \overline{\mathbf{T}}]_\times + \frac{1}{V_0}\mathbf{n}^i \cdot \int_{\Sigma_{-i}} \mathbf{T} \times ((\mathbf{l} + \mathbf{a}_i)\, d\Sigma_{-i}\mathbf{a}_i \cdot\cdot\, \partial_{\mathbf{s}}\partial_{\mathbf{s}}\mathbf{S}) + \frac{1}{V_0}\int_{V_0} \rho_0(\mathbf{L}\times\mathbf{Q} + \mathbf{C})\, dV_0 = \frac{1}{V_0}\int_{V_0} \rho_0(\mathbf{L}\times\dot{\mathbf{u}} + \boldsymbol{\Theta}\cdot\boldsymbol{\omega})^{\cdot}, \quad (3)$$

where $\overline{\mathbf{M}} = \mathbf{a}_i\mathbf{n}^i \cdot \frac{1}{V_0}\int_{\Sigma_{-i}} \mathbf{M}\, d\Sigma_{-i} - \frac{1}{V_0}\mathbf{a}_i\mathbf{n}^i \cdot \int_{\Sigma_{-i}} \mathbf{T} \times ((\mathbf{l}+\mathbf{a}_i)\, d\Sigma_{-i} \cdot \partial_{\mathbf{s}}\mathbf{S})$ is the "first Piola-Kirchhoff macro-couple stress tensor", $\mathbf{L}$ and $\mathbf{l}$ are the local co-ordinate of a subparticle within the cell in actual and reference configuration, respectively. In the law of balance of torque we see an additional term, which appears because the cell is deformable.

MICROSTRUCTURAL APPROACH

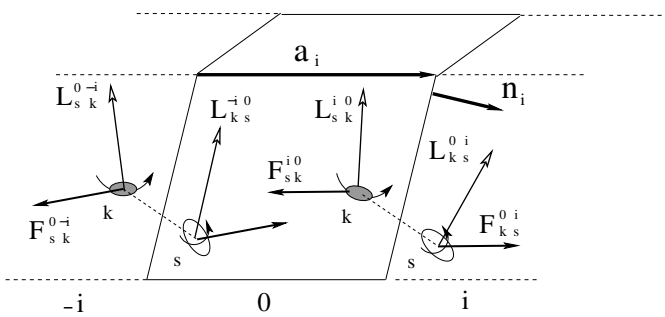

Figure 2. A cell of a crystal. Discrete model

Expansion in macro-co-ordinates

Let $\mathbf{F}_{\ s\ k}^{0\ -i}$ be a force acting from the subparticle s belonging to cell 0 (under consideration) upon a subparticle k belonging to cell $-i$ (obtained by translation of a cell 0 with the translation vector $-\mathbf{a}_i$), and $\mathbf{L}_{\ s\ k}^{0\ -i}$ be a corresponding torque, $\mathbf{R}_s^0$ be a radius-vector of a subparticle s from a cell 0 etc. (see Fig. 2). Using the periodicity of the crystal in the reference configuration, the assumption that forces and torques change smoothly with the change of a cell number, and the balance of forces and torques for a cell, we obtain, expanding in the "macro-co-ordinates",

$$\partial_{\mathbf{s}} \cdot \mathbf{a}_i \sum_{s,k} \mathbf{F}_{\ s\ k}^{0\ -i}/V_0 + \rho_0\mathbf{Q} = \rho_0\ddot{\mathbf{S}}, \quad (4)$$

(so we conclude that $\overline{\mathbf{T}} = \mathbf{a}_i \sum_{s,k} \mathbf{F}_{\ s\ k}^{0\ -i}/V_0$), and

$$\partial_{\mathbf{s}} \cdot \overline{\mathbf{M}} + [(\partial_{\mathbf{s}}\mathbf{S})^\top \cdot \overline{\mathbf{T}}]_\times - \frac{1}{V_0}\sum_{s,k} \mathbf{a}_i(\mathbf{r}_k^0 - \mathbf{r}_C) \cdot\cdot\, (\partial_{\mathbf{s}}\partial_{\mathbf{s}}\mathbf{S}) \times \mathbf{F}_{\ s\ k}^{0\ -i} + \rho_0\mathbf{C}^C = \frac{1}{V_0}\sum_{s\in\Omega}((\mathbf{R}_s^0 - \mathbf{S}) \times m_s\dot{\mathbf{R}}_s^0 + \boldsymbol{\Theta}_s \cdot \boldsymbol{\omega}_s)^{\cdot}. \quad (5)$$

where $\overline{\mathbf{M}} \overset{\text{def}}{=} \frac{1}{V_0}\sum_{s,k} \mathbf{a}_i(\mathbf{L}_{\ s\ k}^{0\ -i} + (\mathbf{R}_k^0 - \mathbf{S}) \times \mathbf{F}_{\ s\ k}^{0\ -i})$. Thus we have the expression for macro stress and couple stress tensors via forces and torques. This method is analogous to the one suggested in [3] for lattices with translational degrees of freedom of particles.

Expansion in micro-co-ordinates

To model forces and torques between subparticles we consider a sufficiently general law of interaction between two subparticles, based on the formula of the point-point interaction between two rigid bodies of general shape: [2]. Particular cases of this formula give, for example, electrostatic, gravitational, or the van der Waals interaction. We obtain the expressions for the force and torque between two sub-particles and expand them in the "micro-co-ordinates". We find out that strain tensors introduced in [4], participate in these complex expressions. Substitution of these expressions into equations (4), (5) completes the passage from the discrete to continuous model.

References

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