Discontinuity Waves in a Continuum with Lattice Microstructure

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Abstract

We study singular surfaces in continua with microstructure; a propagating discontinuity of the microstructure represents a phase transition wave.

Kotchine's theorem gives the local balances of mass, momentum, energy and entropy on singular surfaces in the form of jump conditions, but the case of the micro-momentum is rather different: micro-forces at opposite sides of a discontinuity of the microstructure do not belong to the same linear space.

We deal with the problem of finding which local condition, if any, a discontinuity of micro-tractions has to fulfill. The solution we give is valid for instance when the field of microstructures has a piece-wise pattern like the tessellation of grains in a polycrystal.

1 Introduction

In [2] and [3] the authors deal with discontinuity surfaces in continua with microstructure within the hypothesis of continuity of the microstructure across the surface. Moving discontinuities of the material properties, represented by jumps of the internal variables in classic continua, are studied in [4].

We bring together the two problems and, dealing with continua with microstructure, we focus on possible discontinuities of this field (and thus of the material properties related to it).

Applications pertain *e. g.* to polycrystals modeled as continua endowed with a piece-wise constant crystal orientation function; the surfaces that the jumps of the microstructure are assumed to identify model the interfaces between grains. Macroscopic observations induce us to look at these surfaces as regular but not necessarily material (grain growth or sintering offering examples of non material evolutions of them) and at the microstructure as uniform within each grain.

2 Background

We model a polycrystal as a continuum with microstructure as suggested in [1].

The microstructure, in this case, models a crystal lattice with variable orientation in space, and thus it is an element of a sub-group of rotations of the Euclidean space modulo the symmetries of that lattice. As the particular nature of the crystals will be of no importance here, we choose to represent microstructures through orthogonal tensors and endow the body with a function $M(x,\tau) \in Orth^+$—with $x \in \mathcal{E}$ present

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position of material points in the Euclidean space and τ time. The tangent space at M is $T(M) \equiv \{WM \mid W \in Skw\}$ with Skw space of skew-symmetric tensors.

Grain's boundaries can be modeled as surfaces of discontinuity of this microstructure; they have no mass, momentum, energy or entropy content, they support no external action either, but they may incidentally not follow the material movement. We let Γ denote such a surface.

We introduce the following fields on the present configuration: density ρ, material velocity u, grain boundaries' velocity v ($v = u$ at a place x and time τ if and only if Γ follows the underling matter there and then), Cauchy's stress T, heat flux q, temperature θ, internal energy's and entropy's density respectively ϵ and ς, body forces b, heat supply in the bulk ι. We let κ and χ denote respectively the density per unit mass of the kinetic energy and co-energy of the microstructure, $B \in T^*(M)$ the density per unit volume of the external micro-force, $Z \in T^*(M)$ that of the equilibrated micro-force, $\mathrm{s} \in Lin(\mathcal{V}, T^*(M))$ (with $\mathcal{V}$ translations of $\mathcal{E}$) the micro-stress tensor.

We adopt the usual notation and definition for the discontinuity of a field $[\![a]\!] := a^+ - a^-$, where the suffix denotes the limits of the function a approaching Γ from either sides.

On singular surfaces the conditions corresponding to the balance of mass, momentum, energy and entropy are given by Kotchine's theorem (*cfr* [5]). They can be made concise introducing the time rate of mass crossing the unit surface of the discontinuity in the present configuration—a field defined on Γ starting from the conservation of mass—$\mu := \rho^+(u^+ - v) \cdot n = \rho^-(u^- - v) \cdot n$:

$$\mu[\![u]\!] = [\![T]\!]n \tag{1}$$

$$\mu[\![\epsilon + \frac{u^2}{2} + \kappa]\!] = [\![-q + T^T u + \mathrm{s}^T \dot{M}]\!] \cdot n \tag{2}$$

$$\mu[\![\varsigma]\!] \geq [\![\theta^{-1} q]\!] \cdot n \tag{3}$$

(note that s^T has to be read in the sense of the equality $n \cdot \mathrm{s}^T \dot{M} = \dot{M} \cdot \mathrm{s}n$).

To write the missing condition for the balance of micro-momenta we have to come back to the demonstration of the above mentioned theorem.

3 Balance of micro-momentum on singular surfaces

Let us look at an arbitrary subdomain V^*, presently occupied by part of the body, that the discontinuity surface Γ cuts into two parts together with its boundary ∂V^*. The usual notations V^{*-}, V^{*+}, ∂V^{*-}, ∂V^{*+}, Γ^- and Γ^+ are adopted.

A sufficient condition to go through the classic demonstration of Kotchine's theorem is that the microstructure remains homogeneous during the process on either sides of Γ. Then, following V^{*+} during its motion, we have the global balance of micro-momentum:

$$\int_{V^{*+}} \rho[(\frac{\partial \chi}{\partial \dot{M}})^{\cdot} - \frac{\partial \chi}{\partial M}]\, dV_\tau = \int_{V^{*+}} (B - Z + \mathrm{div}\,\mathrm{s})\, dV_\tau \quad \Rightarrow$$

$$\frac{d}{d\tau}(\frac{\partial \chi}{\partial \dot{M}} \int_{V^{*+}} \rho\, dV_\tau) = \int_{\partial V^{*+}} \mathrm{s}n\, dS_\tau + \int_{V^{*+}} (B - Z)\, dV_\tau + \frac{\partial \chi}{\partial M} \int_{V^{*+}} \rho\, dV_\tau + Z^{*+} \tag{4}$$

where $Z^{*+}(\tau)$ is the total micro-force that the microstructure of V^{*-} exerts on that of V^{*+}:

$$Z^{*+} = \int_{\Gamma^+} \mathrm{s}n\, dS_\tau - \frac{\partial \chi}{\partial \dot{M}} \int_{\Gamma^+} \rho(u - v) \cdot n\, dS_\tau \tag{5}$$

To state that the micro-action Z^{*+} of V^{*-} on V^{*+} equilibrates the micro-action Z^{*-} of V^{*+} on V^{*-}—however we take V^*, as far as the assumed topology of the intersection with Γ holds— we need to choose a reference linear space where this statement can be expressed. There is no natural choice of the kind and an objectivity requirement has to be introduced accordingly.

Rotating both Z^{*+} and Z^{*-} in the dual space of skew-symmetric tensors Skw^*—which is co-tangent to $Orth^+$ at its neutral element—the statement of equal action and reaction writes:

$$\begin{aligned} &\int_{\Gamma^+} sn\, dS_\tau (M^+)^T - \frac{\partial \chi}{\partial \dot{M}}(M^+)^T \int_{\Gamma^+} \rho(u-v)\cdot n\, dS_\tau \quad = \\ &\int_{\Gamma^-} sn\, dS_\tau (M^-)^T - \frac{\partial \chi}{\partial \dot{M}}(M^-)^T \int_{\Gamma^-} \rho(u-v)\cdot n\, dS_\tau \end{aligned} \tag{6}$$

Thanks to the arbitrary choice of V^* and to the definition $n := n^+ = -n^-$, the local jump condition for the microstructure at every regular point of Γ ensues:

$$[\![snM^T]\!] = \mu[\![\frac{\partial \chi}{\partial \dot{M}} M^T]\!] \tag{7}$$

The choice of the reference orientation for the orthogonal tensors is immaterial to this result as proved by replacing M with $RM\ \forall R \in Orth^+$ in equation (7), therefore invariance is fulfilled.

4 Conclusions

We have written the jump condition for the micro-stresses when the microstructure represents a crystal lattice that is uniform at the different sides of a discontinuity surface (*cfr* (7)).

The same approach can be followed in dealing with other kind of microstructures, especially when a finite change of the microstructure gives only a finite rotation of its tangent space.

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