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ON GURTIN-MURDOCH MODEL OF MATERIAL SURFACE

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Material surface model

The Gurtin and Murdoch (G-M) theory of material surfaces, [1], describes free surface (or interface) effects in solids within the framework of elasticity. These effects include presence of the surface residual stresses and modification of the surface properties, comparing with those of the bulk material. They occur as a result of different molecular (or atomic) environment existing on the boundary versus that in the interior, which changes electronic and mechanical interactions between the molecules (atoms), [2]. The surface effects associated with residual stresses and changed elastic properties are negligible in solids unless the surface radii of curvature are sufficiently small, as they are in the case of nano-composites. Consequently, the emerging possibilities of various technological applications of nano-composites spurred significant interest in their analysis and, thus, in G-M theory.

In the original G-M theory the material surface is essentially an elastic membrane adhering to the bulk material and possessing its own, independent of the bulk, constitutive equations. The key element of it is therefore the definition of the surface stress tensor $\boldsymbol{\sigma}_S$. With this tensor defined in terms of surface deformation, the mechanical problem is described by the equation of the material surface

$$[\![\mathbf{u}(\mathbf{x})]\!]_S = \mathbf{0}; \quad [\![\boldsymbol{\sigma}(\mathbf{x})]\!]_S \cdot \mathbf{n}(\mathbf{x}) + \mathrm{div}_S\ \boldsymbol{\sigma}_S(\mathbf{x}) = \mathbf{0}, \qquad (1)$$

coupled with the usual equations of elasticity within the bulk of the material and with the appropriate boundary conditions. In the above equation the subscript *S* represents the material surface, div_S stands for the surface divergence operator, $\mathbf{n}$ is the unit vector normal to *S*, $\boldsymbol{\sigma}$ denotes the stress tensor in the bulk of the material and $[\![\cdot]\!]_S$ indicates the jump of the quantities enclosed in the brackets across the surface.

Development of surface stresses

As clearly argued in [2] (in complete agreement with the usual logic justifying appearance of residual stresses), if the surface layer could be separated from the bulk while retaining all modified intermolecular interactions, its stress-free configuration would be different than the surface of the stress-free bulk material. Thus, in accordance with the kinematic compatibility between the material surface and the bulk material expressed by Eq. $(1)_1$, one can write

$$\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_i; \quad \mathbf{F}\big|_S = \overline{\mathbf{F}}\big|_S, \qquad (2)$$

where $\overline{\mathbf{F}}$ and $\mathbf{F}$ are the deformation gradients of the bulk material and of the material surface, respectively, considering the bulk stress-free configuration as initial for the entire system; $\mathbf{F}_i$ is the material surface deformation gradient describing transition from the initial configuration to the stress-free configuration of that surface; $\mathbf{F}_e$ is the surface deformation gradient associated with development of stresses. It is assumed here that all of the surface deformation gradients are "three-dimensional", and such that they transform the surface unit normal vectors associated with the corresponding configurations into one another; the vectors tangent to the surface are transformed by $\overline{\mathbf{F}}$ and $\mathbf{F}$ identically (cf. Eq.$(2)_2$). With this understanding of the surface deformation gradients one can write

$$\boldsymbol{\sigma}_S = \boldsymbol{\sigma}_S(\mathbf{F}_e) = \boldsymbol{\sigma}_S(\mathbf{F}\cdot\mathbf{F}_i^{-1}) \overset{def}{=} \boldsymbol{\sigma}_S^{\mathbf{F}_i}(\mathbf{F}), \qquad (3)$$

where the symbol $\boldsymbol{\sigma}_S^{\mathbf{F}_i}$ denotes a function of only $\mathbf{F}$ for any fixed $\mathbf{F}_i$. For convenience, the stress tensor $\boldsymbol{\sigma}_S$ is also understood as "three-dimensional" with vanishing normal components.

Comments on the surface stress formula

Several issues associated with Eq. (3), will be discussed during the presentation. In particular:

1. How should one define the surface residual stresses? This is important when those stresses are needed in calculations based on the G-M model and when their value is obtained, for example, experimentally. In [1] these stresses are defined as $\boldsymbol{\sigma}_S^0 = \boldsymbol{\sigma}_S^{\mathbf{F}_i}(\mathbf{I}) = \boldsymbol{\sigma}_S(\mathbf{F}_i^{-1})$, with $\mathbf{I}$ being the identity tensor. This is one possible definition, but the resulting surface residual stresses are then associated with the stress-free bulk material and, in general, violate Eq.$(1)_2$. Such definition appears to be in agreement with explanation offered in [2] and it is used in all calculations based on G-M model known to the Authors. However, some experimental measuring techniques may, in fact, be providing residual stresses in the configuration that obeys Eq. $(1)_2$ (see reference to Nicholson in [2]).
2. How should the material frame indifference and isotropy be defined in the context of Eq.(3)? In [1] it is assumed that both of those notions apply to function $\boldsymbol{\sigma}_S^{\mathbf{F}_i}(\mathbf{F})$ of Eq. (3) which results in $\boldsymbol{\sigma}_S^{\mathbf{F}_i}(\mathbf{Q}\cdot\mathbf{F}\cdot\mathbf{Q}^T) = \mathbf{Q}\cdot\boldsymbol{\sigma}_S^{\mathbf{F}_i}(\mathbf{F})\cdot\mathbf{Q}^T$ valid for every orthogonal $\mathbf{Q}$ and every $\mathbf{F}$. Assuming $\mathbf{F}=\mathbf{I}$ this yields $\boldsymbol{\sigma}_S^0 = \mathbf{Q}\cdot\boldsymbol{\sigma}_S^0\cdot\mathbf{Q}^T$, which implies that $\boldsymbol{\sigma}_S^0 = f(\mathbf{F}_i^{-1})\mathbf{I}$ with $f(\mathbf{F}_i^{-1})$ being a scalar function of second order tensors. Even though postulating that $\boldsymbol{\sigma}_S^{\mathbf{F}_i}(\mathbf{F})$ be isotropic is theoretically acceptable, the resulting conclusion seems unnecessarily restrictive for solid surfaces, [2]. Yet, it is ubiquitous in the analyses based on G-M model. It will be shown during the presentation that assumption of $\boldsymbol{\sigma}_S(\mathbf{F}_e)$ being isotropic does not lead to such a restrictive conclusion.

Some ramifications associated with different possible theoretical assumptions described above will be illustrated by means of simple numerical examples.

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