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Homogenisation of porous thin films and perforated layers: Comparison of analytical and numerical approaches

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ABSTRACT

The mechanical properties of porous thin films and perforated layers are affected by pore content, shape and arrangement. The experimental determination of the in-plane mechanical properties of such materials is challenging, yet reliable data are essential for materials development and component design. Analytical and numerical approaches therefore provide valuable, supplementary tools for evaluating the effect of porosity on the mechanical properties of such materials.

The applicability of both the classical self-consistent method and the Mori–Tanaka approach to the estimation of the effective elastic properties of porous thin films and perforated layers is investigated in this paper. For generic model microstructures with various arrangements of pores, variable pore content and varying matrix Poisson's ratio, the effective elastic properties predicted by the classical self-consistent method and by the Mori–Tanaka approach are quantitatively compared with results obtained by numerical experiments. Based upon this comparison, the range of validity of both the classical self-consistent method and the Mori–Tanaka approach with regard to the different arrangements of pores investigated is defined, and the deviation to be expected if critical values of pore content or inter-pore distance are exceeded and interactions between adjacent pores are occurring is assessed.

1. Introduction

Porous thin films and perforated layers are increasingly used in innovative engineering applications, for example as filters (Kuiper et al., 2002), functional coatings for sensing or catalytic reaction tasks (Van Noyen et al., 2011; Zander et al., 2007), semiconductors in microelectronic devices (Föll et al., 2002), packaging medium for micro-electromechanical systems (Zekry et al., 2010), or to assure the biocompatibility of implants (Buchko et al., 2001). Depending on the intended application, such materials exhibit a wide variability of volume fraction, shape and arrangement of pores, which in turn affects their mechanical properties (Chao et al., 2005; Ha et al., 2010; Jauffrès et al., 2011; Vanstreels et al., 2013). Understanding the relation between pore microstructure and effective mechanical properties therefore plays a key role in successfully implementing these materials in practice.

However, the direct experimental determination of the mechanical properties, such as Young's modulus and Poisson's ratio, of porous thin films and perforated layers involves implications: mechanical indentation tests, which are commonly used to measure Young's modulus, are sensitive to indenter type, penetration depth and substrate influence (Ben-Nissan et al., 2013; Bhushan and Venkatesan, 2005; Hemmouche et al., 2013; Zhou et al., 2011). Due to the limited size of the effectively tested material volume, the local pore structure may seriously

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affect indentation test results (Vanstreels et al., 2013). Advanced optical or acoustic tests, which are used to determine Poisson's ratio, depend upon accurate density measurements and a detailed analysis of the test data to yield reliable results (Flannery et al., 2001; Zhou et al., 2011).

Against this background, analytical homogenisation approaches provide valuable tools for accompanying the interpretation of test results and evaluating the effect of porosity on Young's modulus and Poisson's ratio of porous thin films and perforated layers, stimulating and speeding up the process of materials development and component design. To be of practical use, such approaches need to be able to accurately capture interaction effects arising from the particularly small inter-pore distances of these materials.

In the present paper, this issue is investigated with regard to both the classical self-consistent method (SCM) initially suggested by Hershey (1954) and Kröner (1958) and the Mori–Tanaka approach (MT) described by Tanaka and Mori (1972). The SCM and the MT represent analytical homogenisation approaches capable of accounting for pore content and interaction effects between neighbouring pores, lending themselves to the computation of the Young's and shear moduli and Poisson's ratios of porous thin films and perforated layers. To further advance the understanding of the impact of pore content and arrangement, as well as inter-pore distance, on the applicability of the SCM and the MT to the homogenisation of such materials, the following open questions are addressed:

- How are porosity and inter-pore distance correlated?
- What are the intervals of porosity and inter-pore distance over which the SCM and the MT yield acceptable results?
- How does the Poisson's ratio of the bulk material influence the results of the SCM and the MT?

These questions were investigated in a series of numerical experiments on generic, planar microstructure models with circular pores. The microstructure models were generated by means of a specifically developed software tool, which allows to create virtual microstructures with varying pore content and arrangement. Microstructure models with square, rhombic and random arrangements of pores were studied in order to cover the range of pore configurations commonly found in reality.

In order to evaluate the validity of predictions obtained by the SCM and the MT, the effective elastic properties estimated by the SCM and the MT for different levels of porosity and varying Poisson's ratio of the bulk material were quantitatively compared with results obtained by finite element analyses of these microstructure models in conjunction with a numerical homogenisation approach (Anthoine, 1995; Michel et al., 1999). To identify a correlation between porosity and inter-pore distance, the inter-pore distances of microstructure models with square and rhombic pore structure, as well as the average inter-pore distances of several thousand random microstructure models found by a Monte-Carlo simulation, were related to their pore content. These investigations led to clear guidelines on the applicability and range of validity of both the SCM and the MT with regard to the homogenisation of porous thin films and perforated layers with square, rhombic and random pore configurations.

2. Analytical homogenisation approach

In general terms, porous thin films and perforated layers represent a variant of inhomogeneous two-phase materials, which are composed of constituents with different mechanical properties, namely a matrix phase and inclusions or, in the case of vanishing stiffness, pores. In order to treat such materials within the framework of continuum mechanics, the identification of their effective mechanical properties, which are governed by the volume fraction, shape, arrangement and mechanical properties of the constituent phases, is required. The effective elastic properties are commonly found by homogenisation, which involves evaluating the mechanical response of a finite, generic section of the inhomogeneous material, a so-called Representative Volume Element (RVE) (Hill, 1963). In order to formulate the constitutive equation for the RVE domain, the complex local stress and strain fields within the constituent phases are calculated individually, and their contribution to the overall stress and strain state is accounted for by volume averaging. The resulting effective elasticity or compliance tensors represent an equivalent homogeneous continuum, which replaces the initial inhomogeneous microstructure of the RVE domain.

2.1. Basic relations

The main aspects of the analytical homogenisation of porous thin films and perforated layers are outlined in this section. The following considerations are limited to linearly elastic materials that exhibit a matrix-inclusion-type microstructure with a homogeneous matrix domain Ω_m and an inclusion domain $\Psi = \bigcup_{i=1}^{n} \Psi_i$, which represents the union of n homogeneous inclusions, or, in the case of vanishing stiffness, pores Ψ_i distributed over Ω_m. The inclusions Ψ_i are assumed to be of similar shape and orientation and to have identical elastic properties. The domain $\Omega = \Omega_\mathrm{m} \cup \Psi$ constitutes a Representative Volume Element (RVE) of a porous thin film or perforated layer, as shown in Fig. 1.

The constitutive equation of the matrix phase reads

$$\overline{\boldsymbol{\sigma}}^{\Omega_\mathrm{m}} = \boldsymbol{C}^{\Omega_\mathrm{m}} : \overline{\boldsymbol{\varepsilon}}^{\Omega_\mathrm{m}}, \tag{1}$$

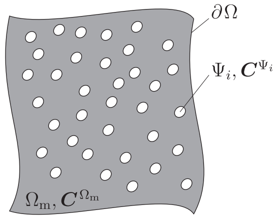

Fig. 1. Schematic representation of a RVE for a porous thin film or perforated layer with matrix domain Ω_m and n homogeneous inclusions Ψ_i.