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Multi-field asymptotic homogenization approach for Bloch wave propagation in periodic thermodiffusive elastic materials

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Abstract. Multi-field asymptotic homogenization methods are proposed to describe the behaviour of periodic Cauchy materials subject to several physical phenomena, focusing on thermodiffusion. The resulting homogenized models provide the overall constitutive tensors and overall inertial terms. Moreover, they allow one to investigate the complex band structures associated with damped Bloch waves travelling in periodic materials, avoiding the challenging computations needed by the adoption of micromechanical approaches.

1. Introduction

Periodic composite materials subject to thermodiffusive phenomena [1,2] are of great interest for many important engineering and technological applications. For example, several renewable energy devices, energy harvesters, battery devices, like lithium-ion batteries and solid oxide fuel cells (see Figure 1), are characterized, among the others, by periodic configurations possessing many phases made of different materials. Furthermore, since high operational temperatures can be reached in such devices, and intense particle fluxes are needed to sustain their electrical current, their components can be subject to severe thermomechanical stresses, as well as to stresses induced by the intense particle diffusion and to thermal-shock waves, which can compromise an adequate performance of these devices. For such reason, a characterization of their overall constitutive equations can be extremely useful to predict these phenomena, to ensure a successful manufacturing of such systems and their reliability, and for the optimal design of innovative materials used to build these devices.

Multi-field asymptotic homogenization methods are rigorous and consistent tools for determining the overall constitutive tensors characterizing the behaviour of the periodic material, also in the presence of several physical phenomena, in a synthetic and accurate way [3-9]. The homogenized model provides a useful tool for the damped wave propagation analysis in both bounded and unbounded domains, avoiding the challenging computations required by micromechanical approaches. Moreover, the nonlocal homogenized models provide an accurate description of the acoustic behaviour of periodic Cauchy materials. By increasing the order of the nonlocal continuum in which proper nonlocal constitutive and inertial terms are involved, they allow one to approximate in a consistent way the complex frequency spectrum (complex band structure) of materials with periodic microstructures in the high frequency and short wavelengths domain.

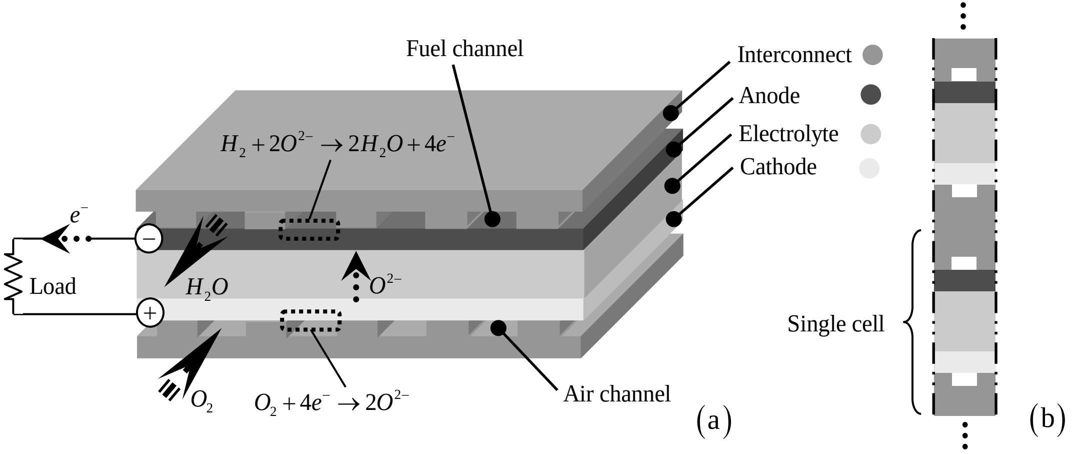

Figure 1: (a) Solid oxide fuel cell (SOFC); (b) Schematic multi-layer SOFC device (adapted from [4]).

2. Multiscale modelling of periodic Cauchy materials vs. local or nonlocal average governing equations

Dynamic microscopic field equations, expressed in terms of the physical and mechanical properties of the periodic microstructure, are asymptotically expanded, obtaining *recursive differential problems* (formulated in terms of microscopic variables, i.e. microscopic displacement, temperature and chemical potential fields), defined on the periodic cell A of characteristic size ε, which is representative of the material. Imposing the A-periodicity solvability conditions for recursive differential problems, suitable down-scaling relations are determined. They relate the microscopic variables to macroscopic ones and to their gradients, by means of A-periodic perturbation functions. Such perturbation functions depend exclusively on geometrical and physical-mechanical properties of the microstructure, and are determined by solving suitable *hierarchical cell problems.* These are obtained by inserting, in a suitable way, the different orders of the down-scaling relations (expressed as asymptotic expansions in ε) into the recursive differential problems expressed in terms of the microscopic variables. The solvability conditions of the hierarchical cell problems in the class of A-periodic solutions allow one to obtain the macroscopic governing equations of a homogeneous equivalent continuum, or rather to obtain higher order approximations of microscopic field equations, by considering nonlocal terms of the averaged field equations of infinite order. Appropriate time-dependent down-scaling and up-scaling relations correlating the microscopic fields to the macroscopic displacement, temperature and chemical potential fields are consistently determined, and the effects of the material inhomogeneities are described by perturbation functions. In particular, a closed form of the overall constitutive tensors and of the overall inertial terms is obtained, involving the perturbation functions and the microscopic constitutive tensors.

Finally, the complex band structure associated with damped Bloch waves travelling in periodic thermodiffusive elastic materials is analytically determined, applying the Fourier-Bloch transform method in accordance to Floquet-Bloch theory (see Figure 2 for some curves obtained using this procedure). The actual complex frequency spectrum in the low frequency and long/medium wavelengths domain is compared with the one obtained using the nonlocal continuum derived from a second order homogenization scheme. Moreover, its asymptotic approximation, also in the high frequency and short wavelengths domain, is expressed in closed form through perturbation techniques.

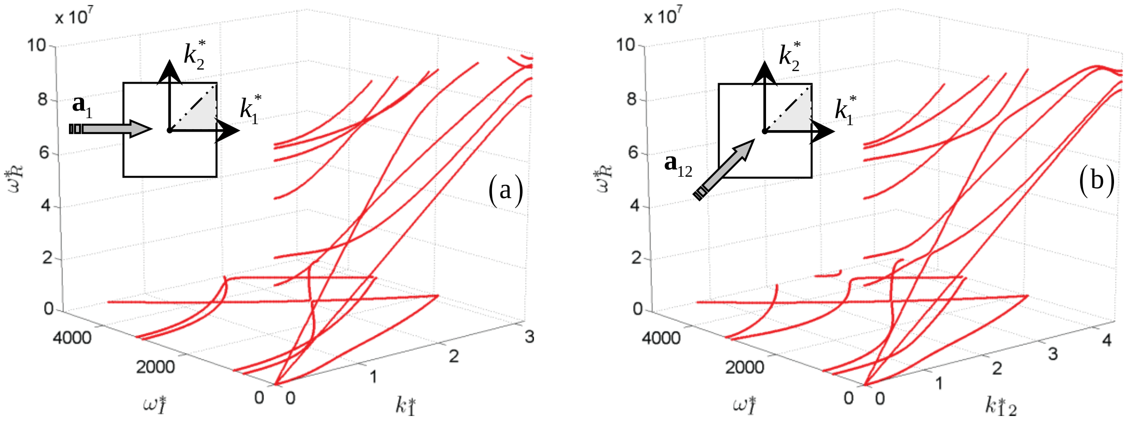

Figure 2: Complex band structure of the thermodiffusive material obtained via the Fourier-Bloch transform method. Wave propagation along: (a) $\mathbf{a}_1$ and (b) $\mathbf{a}_{12}$ directions.

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