An Iterative Routine for Macroscopic Modeling of Electromagnetic, Thermal, and Mechanical Phenomena in Microwave Sintering

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***Abstract*— Adequate computer modeling of microwave sintering is commonly considered to be a serious challenge because of changing geometry of the processed powder compacts. This paper addresses the problem of numerical simulation of microwave sintering at a macroscopic scale. The developed approach involves two software packages: *QuickWave-3D*, a simulator that uses the conformal finite-difference time-domain algorithm for the analysis of electromagnetic wave propagation, and *Abaqus*, a finite element solver for coupled thermal transfer and mechanical deformation. Principles behind this modeling approach are reported, along with a computational implementation and an illustration of the joint operation of coupling of the relevant solvers, via simulation of a specimen (powdered zirconia) in a single mode microwave furnace.**

Keywords – coupling, FDTD, FEM, microwave sintering, multiphysics modeling.

I. INTRODUCTION

Microwave sintering is a promising technology that, in properly designed systems, could allow for energy savings and faster processing of ceramic and metallic powders. The main benefit in comparison with traditional sintering (via conventional heating) is that heat is generated in the bulk of specimen, so higher heating rates can be possible without excessive temperature gradients, which in turn leads to finer microstructure and enhanced material properties. However, in order to become an efficient industrial technology, microwave sintering should be made better controllable, and this must include a means for predicting the effect of thermal runaway, which frequently occurs during microwave sintering, as the loss factor of most ceramic materials drastically increases with temperature.

Modeling of microwave sintering could clarify the effects of many phenomena occurring in the course of sintering. As density has a great influence on thermal conductivity and dielectric properties, Maxwell's equations, heat conduction equations, and a mechanical model describing the constitutive behavior of the powder (including densification) are, in reality, strongly coupled. An efficient and accurate model operating at a macroscopic scale should involve an appropriate method of accounting for this coupling. Although multiphysics modeling of microwave heating has long been routinely used [1-9], coupling with a mechanical solver has not yet been introduced. The chief reason for this lies in the principal difficulty of performing accurate electromagnetic analysis of a microwave scenario with geometry of the processed material changing in time due to mechanical deformation and densification. Different numerical techniques have been found to be most suitable for electromagnetic phenomena occurring during microwave thermal processing and for mechanical deformation occurring during conventional sintering: finite-difference time-domain (FDTD) [10] and finite element method (FEM) [11] respectively.

The use of two different numerical techniques requires development of a computational environment in which the two techniques—featuring conceptually different meshes—would operate jointly in the framework of an efficient iterative procedure running electromagnetic, thermal and mechanical solvers successively, before starting electromagnetic analysis again in a geometrically modified scenario. This challenging problem has been approached in [12] through an attempt to create an FDTD-FEM interface based on interpolation of data to be transferred between the finite-difference mesh associated with the thermal solver and the finite element mesh involved in mechanical model. However, this interpolation approach was found to have very limited capability because of quickly accumulating error during multiple iterations between the solvers.

In this paper, we address the problem of interfacing the FDTD and FEM simulators from a different perspective. We present a computational scheme implementing joint operation of an FDTD electromagnetic solver and an FEM software performing coupled thermal and mechanical simulation. The developed routine is based on the coupling of two software packages: *QuickWave-3D* for the electromagnetic part and *Abaqus* for the thermal and mechanical parts. In this work, we present features of both software packages, explain how we couple them for a comprehensive simulation of microwave sintering, and present an example of an illustrative numerical simulation.

II. CONCEPT OF A FULLY COUPLED MODEL

Microwave sintering is a complex multiphysics phenomenon involving electromagnetic, thermal, and mechanical processes that are strongly coupled and, moreover, operate on different time scales. The physics of microwave sintering suggests a concept of numerical modeling that simulates each

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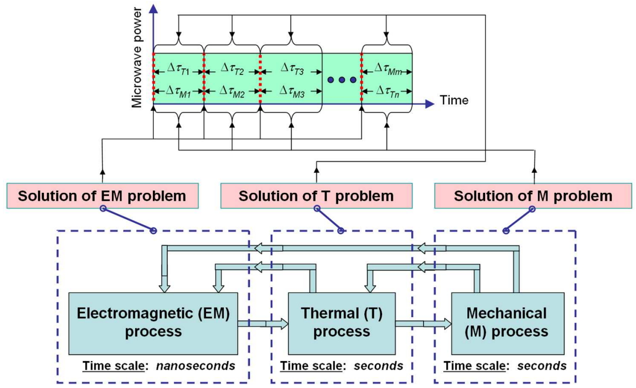


Figure 1. Principal aspects of the concept of comprehensive numerical solution for modeling of microwave sintering.; $\Delta\tau_{Ti}$ is a time stepin mnicrowave heating, $\Delta\tau_{Mi}$ is a time step in structural deformation.

of the three main physical processes using respective numerical solvers, with coupling implemented through an iterative procedure that employs an appropriate time scale, as illustrated by the flow chart in Fig. 1.

A. Electromagnetic Modeling

QuickWave-3D (*QW-3D*) is a three-dimensional electromagnetic simulation package that uses the conformal FDTD algorithm to solve boundary value problems in high frequency electromagnetics [13]. It includes a range of options for curved boundaries, media interfaces, modal excitation, and parameter extraction, and can be applied to various problems including calculation of heating patterns for microwave power applications, with accurate and fast display of instantaneous, time-maximum and time-averaged patterns of fields and dissipated power.

B. Thermal and Mechanical Modeling

The *Abaqus* software suite integrates implicit and explicit finite element analysis to solve a wide variety of multiphysics problems, including nonlinear, large-scale linear, and contact problems [14]. In particular, *Abaqus* includes a procedure for implementing fully coupled constitutive thermal and mechanical equations in a transient coupled temperature-displacement procedure where the heat transfer equations are solved using a backward-difference scheme, and the coupled system is solved using Newton's method. The mechanical constitutive equation is implemented through the CREEP subroutine, and has used in [15-17] to simulate conventional sintering. One particular feature of *Abaqus* that is exploited in our coupled model is the ability to import a user-defined mesh.

C. Comprehensive Model of Microwave Sintering

A comprehensive model of microwave sintering that uses these two software packages must account for the fact that *QW-3D* uses the FDTD algorithm, while *Abaqus* uses the finite element method. In particular, these two numerical methods impose different requirements on the mesh discretizing the simulated system: the mesh automatically generated by a FEM solver employs irregularly-shaped hexahedral elements, where

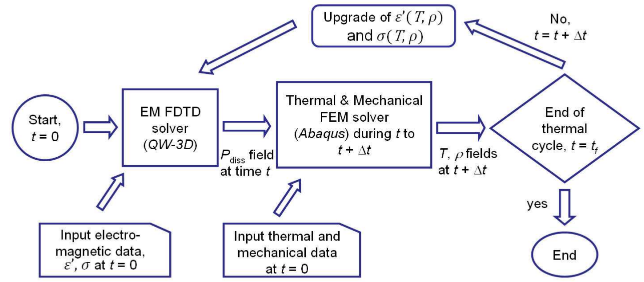


Figure 2. Concept of a fully coupled, comprehensive numerical model of microwave sintering. t_f – time to sinter, P_{diss} – field of dissipated power, T – temperature, ρ – density, σ – electric conductivity, ε' – dielectric constant.

that generated by an FDTD solver uses Cartesian cells. As the solutions exported by the solvers are discrete values taken at the nodes of cells and elements, a principal problem that must be addressed by a comprehensive model of microwave sintering is how to transfer data between two different meshes.

This problem was addressed in [12], where interpolation and intersection approaches were considered. Using these methods, the error is indeed sufficiently low over a single iteration, but a full simulation of microwave sintering may involve thousands of iterations, and it was determined that the error compounds quite quickly over multiple iterations.

Here, we therefore seek to minimize the need for data transfer between meshes, and to this end, we exploit the feature of *Abaqus* that allows the user to import a predefined mesh. In particular, the coordinates of the mesh generated by *QW-3D* for solutions of the electromagnetic problem are exported directly to *Abaqus*, along with the data on dissipated power evaluated at those coordinates. It is important to note that naturally, an FDTD mesh with Cartesian cells also constitutes an admissible, conforming triangulation for use in an FEM simulation, and so a mesh generated by *QW-3D* can also be used by *Abaqus*.

With this in mind as a necessary feature for the simulation, we propose a concept of the fully coupled model, as shown in Fig. 2, that operates according to the following steps.

1. Initially, the geometry of the cavity and sample is reproduced in *QW-3D*, the geometry is properly meshed, electromagnetic simulation is performed.
2. The geometry of the sample and the Cartesian mesh discretizing it are exported to *Abaqus*, along with the dissipated power field within the sample.
3. *Abaqus* then runs the CREEP subroutine to simulate heat generation, mechanical deformation, and densification of the sample.
4. Material properties are updated in *QW-3D* accordingly with the temperature and density change, to start the subsequent iteration.

III. Illustrative Simulation Example

The fully coupled numerical model of microwave sintering presented in the preceding section has been partially implemented, and we provide here, as an illustrative example, the results of one loop in the iterative procedure, with the coupling and data transfer carried out manually, simulating the sintering

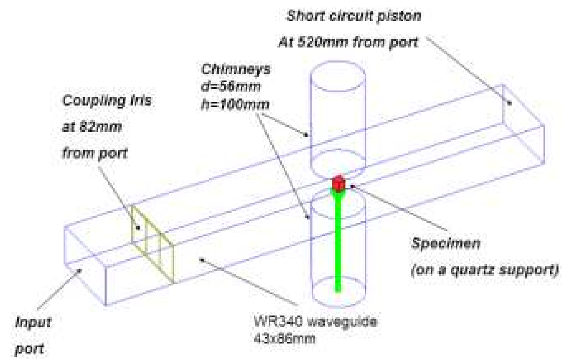


Figure 3. Geometrical characterization of the SIMaP single-mode microwave sintering furnace.

of a powdered zirconia sample in an existing single-mode microwave furnace.

A. *Geometrical Characteristics of the Furnace*

The modeled furnace (Fig. 3) consists of a single-mode resonant cavity as a waveguide with cross-section 86 x 43 mm. In the center of the cavity, there are two vertically oriented, cylindrical chimneys used for placement and monitoring of the sample. A coupling iris and short-circuit piston exist as a mechanism to control the standing wave pattern. The geometrical characteristics of the entire system, including the quartz support on which the sample rests, are reproduced in *QW-3D* and meshed using non-uniform hexahedral cells with maximum size 5 mm in air, 1.5 mm in the quartz support, and 0.5 mm in the sample. The total number of cells was about 920,000. More details about this setup can be found in [18].

B. *Characteristics of Numerical Simulation*

The temperature-dependent electromagnetic and thermal material properties of the zirconia sample used in the electromagnetic simulation were taken from [19] and [9] respectively. The mechanical constitutive equation implemented in the CREEP subroutine comes from [20] where it was developed for modeling sintering of a material whose mechanical properties are different from those of zirconia. Since at this stage of development of a comprehensive modeling tool we are concerned with illustration of the principle of joint operation of electromagnetic FDTD and thermo-mechanical FEM solvers (represented in our consideration by *QW-3D* and *Abaqus*) rather than with an attempt to model mechanical deformation of zirconia undergoing microwave sintering, we find this combination to be instructive, as it allows us to implement the required coupling. In the computation, we assume that the bottom of the specimen is thermally insulated by the quartz support, and radiation conditions with emissivity 0.1 were applied to the other five faces of the specimen.

As according to the plan, geometrical characteristics of the sample were reproduced in an existing *QW-3D* model of the microwave furnace. In order to raise the sample to a temperature high enough so that significant heating would occur as a result of microwave power, a coupled thermal-mechanical analysis was first conducted in *Abaqus* with a mesh identical to the one used in *QW-3D*. This analysis assumed a

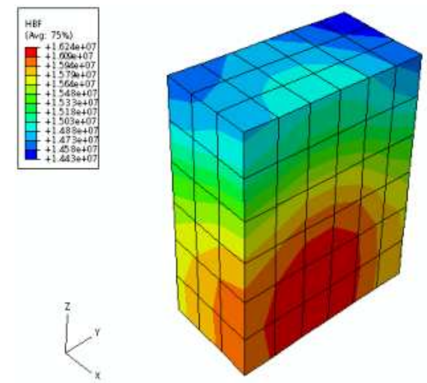
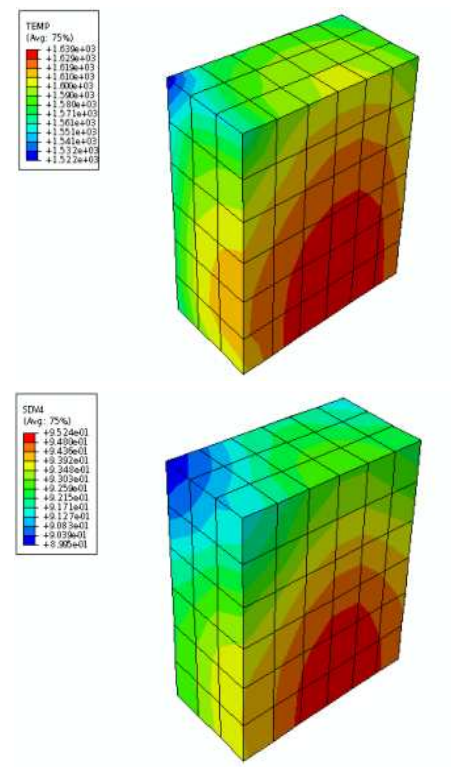


Figure 4. Dissipated power distribution (in W/m^3) in the half-specimen after export from *QW-3D*.



(a)

(b)

Figure 5. Temperature (a) and relative density (b) distributions on the surface of the half-specimen after the end of the second step of the thermal-mechanical analysis.

uniform heat source, linearly increasing within the sample from 0.5 to 8 W/mm^2 over 6000 seconds. The temperature at the end of this step was in the range 1342-1400 °C, and the relative density was in the range 0.63-0.65. The resulting temperature and relative density distributions were processed to calculate an enthalpy distribution, which was used to update the dielectric constant and electric conductivity in *QW-3D*, where EM simulation was subsequently run.

The resulting dissipated power distribution (Fig. 4) was exported to *Abaqus* and a second thermal-mechanical analysis with duration of 4000 s was carried out. The temperature and relative density distributions obtained at the end of this step is shown in Fig. 5, with minimal and maximal temperatures at 1521 and 1639 °C respectively, and relative density in the range 0.90-0.95. Density in this range indicates that the sintering progressed significantly in a heterogeneous way during this step.

IV. Discussion and Conclusion

The possibility of coupling *QW-3D* to *Abaqus* to perform comprehensive modeling of electromagnetic, thermal and mechanical processes occurring during microwave sintering has been demonstrated, and an example illustrating the joint operation of this coupled solver has been shown. The output of this paper therefore suggests that with the development of corresponding *Abaqus* CREEP subroutines for a variety of materials, the proposed concept could be implemented as a practical modeling tool. In this contribution, the export of the field of dissipated power has been shown possible under the condition of geometrically identical FDTD and FEM meshes.

We define the next step in the development of the technique of comprehensive modeling of microwave sintering to be construction of a two-way interface between *QW-3D* and *Abaqus* ensuring a closed, automatic, iterative analysis of electromagnetic, thermal and mechanical processes. The major challenge here is the necessity of flexibly handling information about changing geometry that is simulated by *Abaqus* and should be used as input data by *QW-3D* – this functionality will likely require the condition of geometrically identical meshes to be dropped. In the context of these goals, this paper confirms the validity of the proposed FDTD-FEM concept in comprehensive multiphysics numerical simulation of microwave sintering.

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