

Multiphysics Modelling of a Microwave Furnace for Efficient Silicon Production

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Abstract: Silicon must be extremely pure, above 99.9999% to be used in solar and semiconductor applications. A novel approach to meet this requirement is the use of microwave furnaces and high-purity raw materials without going through successive purification processes. Hence, it is desirable to develop computer simulation methodologies to identify the efficient design of the microwave furnace. This is done by modelling the internal processes taking place within the microwave. For this purpose, the governing equations and boundary conditions are solved for several combinations of materials and geometries. The resulting profiles provide valuable information on performance of the system.

Keywords: Solar Silicon, Microwave Furnace, Radio Frequency, Heat Transfer, Computational Fluid Dynamics

1. Introduction

The demand for silicon as the main raw material in communications and photovoltaics is steadily increasing. The JPM silicon GmbH presents a novel method for the production of solar grade silicon in a microwave oven. This method can specially reduce the energy costs and increase the efficiency of the process. Figure 1 shows a schematic view of the components of the system. Principally, the core of the system is a magnetron, which generates electromagnetic microwaves. The generated waves are transmitted through the waveguide to the reaction chamber or resonator. The reaction chamber holding the sample is the main area for concentration of the electrical field, which heats the sample up. The tuner guarantees better absorption of the microwaves generated by the magnetron. Finally, the system is equipped with a circulator, which dissipates the reflective microwave energy into a water bath as a heat sink in order to protect the magnetron against possible overheating.

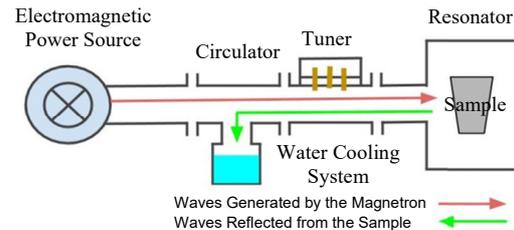


Figure 1. Schematic representation of the microwave system of JPM Silicon GmbH.

Basically, the microwave heating allows for selective heating of certain materials on a volumetric heat input, thus reducing the heat loss through a temperature drop from the inside out, over the conventional processes. Due to the faster warming and shorter residence time, the diffusion of impurities in the sample is also reduced.

In order to optimize the existing processes, knowledge of the three-dimensional temperature distribution and the local heat flux is required. A measurement of the temperature with thermocouples in the microwave process is not possible, since the presence of metallic objects leads to a local elevation of the electromagnetic field. Instead, a numerical model is developed, which depicts the physical, chemical and electromagnetic phenomena of silicon production process. Using COMSOL Multiphysics software a dynamic coupling between the electromagnetic field distribution and the temperature profile can be established, which particularly takes the strong temperature dependency of electromagnetic properties of some materials into account.

In order to increase the efficiency of the system, it is important to identify the relevant influencing parameters and estimate their uncertainties. By variation of the component's materials and the design of the system, the model is optimized and extended for a multicomponent system.

2. Governing Equations in Microwave Heating

The equations that govern microwave heating of a material are Maxwell's Equations, which govern the propagation of the microwave radiation, and the Forced Heat Equations, which govern the absorption and diffusion of heat by the materials.

2.1 Maxwell's Equations

For calculating the heat input in a volume element, the calculation of the electric field (\vec{E}) and the magnetic field (\vec{H}) is required. The Maxwell equations describe the relationship between different electromagnetic field sizes.

$$\begin{aligned}\nabla \times \vec{H} &= \vec{j} + \frac{\partial \vec{D}}{\partial t} \\ \nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t} \\ \nabla \cdot \vec{D} &= \rho \\ \nabla \cdot \vec{B} &= 0\end{aligned}$$

In order to solve the Maxwell equations, additional equations are needed that describe the material dependency behavior. These equations can be simplified as:

$$\begin{aligned}\vec{D} &= \epsilon_0 \cdot \epsilon_r \cdot \vec{H} \\ \vec{B} &= \mu_0 \cdot \mu_r \cdot \vec{H}\end{aligned}$$

Where ϵ_0 and μ_0 describe the electromagnetic behavior in vacuum. It should be noted that the permittivity ϵ_r is a complex quantity, composing of a real (ϵ_r') and imaginary part (ϵ_r'').

$$\epsilon_r = \epsilon_r' + i \cdot \epsilon_r''$$

Where the real part is a measure of the polarizability of a material, while the imaginary part characterizes the quantity of the associated heat release.

2.1 Forced Heat Equations

Thermal Conduction: By means of conduction, the heat is transferred through a medium as a result of interactions between molecules or

atoms. In this form of heat transfer, no microscopic material flow is required, thus it is mainly specified to solid media. For a sufficiently large body, the heat conduction can be calculated through the Fourier's law. This law states that the time rate of heat transfer through a material is proportional to the negative gradient in the temperature and to the area, at right angles to that gradient, through which the heat flows.

$$\vec{q} = -\lambda \text{grad } T = -\lambda \nabla T$$

Thermal Convection: Convective heat transfer is one of the major types of heat transfer between a solid and a fluid. When there exist a temperature difference between a body and a fluid in contact, the heat is transferred from the surface of the body to the fluid by means of conduction. Individual particles of the fluid take the thermal energy and carry it from the surface to into the main stream flow. The general approach to the description and calculation of the heat supplied by convection is:

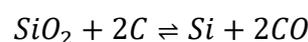
$$\dot{q} = \alpha(T_s - T_\infty)$$

Heat Radiation: In the heat transfer by radiation, no transport medium is required. All bodies can emit energy in the form of electromagnetic radiation. The intensity of this radiation depends on one hand on the temperature of the body and on the other hand, on its nature and geometry. Heat radiation from a solid or a liquid usually possesses a continuous spectrum with a characteristic curve, which can be described by Planck's radiation law. However, gases emit radiation in the range of characteristic line spectrum of the material. The theoretical maximum heat flux of a so-called black body is described by the Stefan-Boltzmann law:

$$\dot{q}_{max} = \sigma \cdot T^4$$

3. Theory

Silicon is the product of the reduction of quartz (SiO₂) with carbon (C) at high temperatures resulting in silicon (Si) and carbon monoxide (CO).



In fact, conventional silicon production methods are not only energy intensive and costly but also experienced operators are required. Furthermore, the produced silicon metal has a purity of 98.5% and has to be refined to reach the required purity of 99.9999%. In today's industry this is done via the gas-phase. Thus, silicon metal forms a gaseous silicon compound with hydrogen chloride. This compound is distilled to high-purity and decomposed afterwards to give solar silicon. The process itself originates in the 1950s and is technically complex and energy intensive. On the contrary, JPM Silicon starts with high-purity raw materials and uses a contamination-free microwave furnace to directly obtain solar silicon. This reduced energy consumption and subsequent refining costs results in low-cost solar silicon.

4. Model Properties

As shown in Figure 2, the structure of the microwave oven can be divided into main three parts: 1) the reaction zone, 2) the waveguide, and 3) the electromagnetic power source.

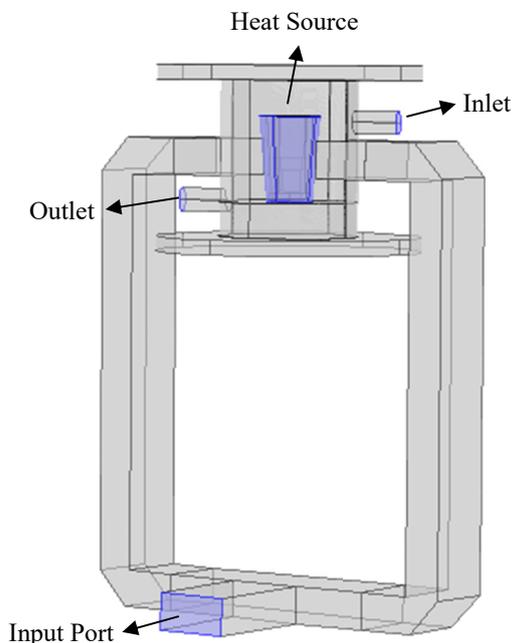


Figure 2. Main components of the microwave system.

The reaction chamber encompasses the crucible, the isolation, the waveguide ports for coupling the microwave field, and the gas inlets or outlets. The reaction zone refers to the area that is in direct contact with the reaction mixture, which must be heated. The waveguide structure is used to transmit the generated electromagnetic field into the resonator chamber. The distribution of the electromagnetic field should be in the way that the predetermined power input is achieved. The maximum power to be provided by the furnace is 2.4 kW at a nominal frequency of 2.45 GHz.

For illustration of relevant processes within the microwave oven, the Heat Transfer (HT) module, the Radio Frequency (RF) module, and the Computational Fluid Dynamics (CFD) module are used. In RF module, the calculation of the electromagnetic field intensity and distribution is carried out, which is originated from the intended port power (p) and the electromagnetic boundary conditions are set according to the Maxwell's Equations. The total dissipated heat through polarization effects is interpreted as volumetric heat source in the HT module. The HT module forms the heat transfer mechanisms in different material types. This constitutes the thermal conduction in solids, the convective heat transport in gaseous media, and the electromagnetic radiation in the form of photons in both transparent and opaque media. The CFD module solves the Navier-Stokes equations, obtaining the gas velocity profile, which will be used by HT module for the calculation of convective thermal losses.

4.1 Material properties

Selection of the proper materials is an important part of the design. An important feature of the design of a microwave oven is that the structural materials should be of high chemical stability in order to prevent unwanted reactions with the reaction mixture. Moreover, the effective insulation materials should be used in order to enable an energy efficient process by minimizing the heat losses. The dimensions of the insulation depend on the geometry of the reaction zone and of the resonator. Basically, selection of the right and optimal combination of materials has enormous effects on the design of the microwave furnace. In order to realize these effects, costly and time-consuming tests should be performed.

However, with the help of numerical simulations, several material combinations can be put to the test for identifying the optimum ones.

6. Results

6.1 Frequency Dependent Electromagnetic Wave Study

The electromagnetic field intensity and distribution inside the resonator chamber and the sample holder are shown in cross section in Figure 3. The wave-like spread of electric field through the waveguide is clearly visible. At the height of the waveguide ports, the electric field is increased relative to the rest of the resonator. Moreover, a field enhancement at the core of the crucible is also observed. This is the ideal height, where the crucible can be located to be heated. However, the electric field strength alone cannot be used as a measure of the heat input in the system. Therefore, a further heat study is required.

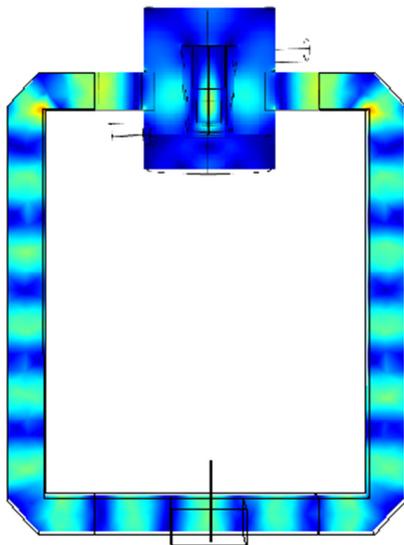


Figure 3. Electric field distribution in the resonator and waveguide.

6.2 Stationary Heat Transfer Study

Figure 4 shows the resulting temperature distribution throughout the resonator chamber. From the electromagnetic study, the hottest point

was expected to be at the core of the crucible, which is totally in agreement with the result from temperature study. Besides, the adjacent insulation layers around the sample were expected to heat up less, due to the comparatively low thermal conductivity, which is also compatible with the result.

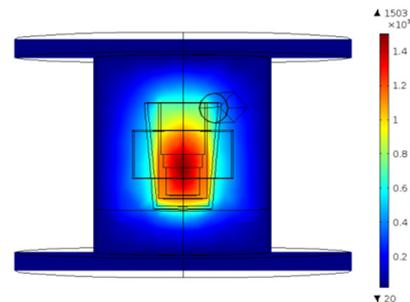


Figure 4. Heat distribution in resonator.

6.3 Stationary Laminar Gas Flow Study

Ideally, the resonator should be filled with an inert gas in order to prevent unwanted reactions like combustion of the sample in presence of Oxygen. In addition, products of gaseous reaction should be eliminated from the resonator to avoid electrical arcs and the generation of plasmas, because this affects the process stability and efficiency.

As shown in Figure 5 no homogeneous velocity profile is made in the resonator chamber. The inert gas flows substantially across the surface of the sample, which later will be deflected by the resonator chamber wall to the bottom. Moreover, only a slight gas flow through the top and bottom areas of the chamber and the areas close to the waveguides ports can be observed.

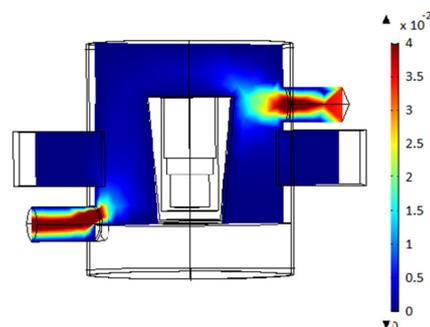


Figure 5. Gas velocity distribution in resonator.

6.4 Optimum Position of the Crucible

The material to be heated in the reaction chamber is located on an insulating plate. In order to investigate the influence of the height of the insulation plate on the electric field distribution, a parametric study of its height is performed. As shown in Figure 6 the height of the insulation plate varies from 30 mm to 40 mm and 50 mm from top to bottom. The results indicate that at the height of 40 mm, the electric field is mainly concentrated in the middle of the crucible, which contains the sample to be heated. However, at higher (50 mm) and lower (30 mm) heights a less strong concentration can be observed. This means, the ideal height of the insulation plate for this geometry is 40 mm.

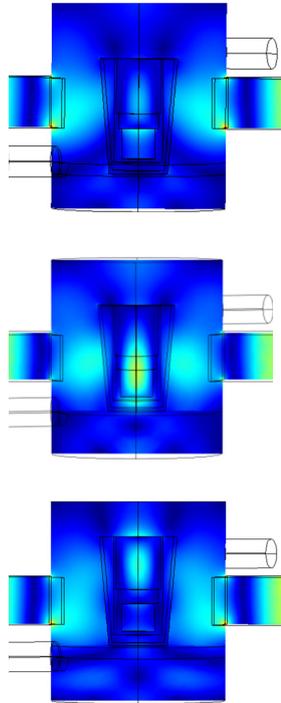


Figure 6. Study of the electric field distribution for different heights of the insulation plate.

7. Conclusions

COMSOL Multiphysics made it possible to simulate the internal processes within the microwave furnace. This includes the calculation of the electromagnetic field intensity and distribution throughout the furnace and the resulting heat inside the reaction mixture through conduction, convection and radiation, followed by calculation of the heat loss of the system. The simulation results could mainly help to identify the optimum design and appropriate materials in order to reach a high-efficiency system.

Table 1: List of abbreviations.

Symbol	Description	Unit
μ_0	Magnetic Field Constant	$4\pi \cdot 10^{-7} \text{ V} \cdot \text{s} / \text{A} \cdot \text{m}$
\vec{B}	Magnetic Flux	Wb
\vec{D}	Electrical Flux Density	C / m^2
\vec{E}	Electric Field	V / m
\vec{H}	Magnetic Field	Tesla
\vec{j}	Current Density	A / m^2
T_∞	Temperature of the External Flow Far Away from the Body	K
T_s	Temperature of the Body in Flow	K
\dot{q}	Heat Flow Rate	W / m^2
ϵ_0	Permittivity of Vacuum	$8.854 \cdot 10^{-12} \text{ A} \cdot \text{s} / \text{V} \cdot \text{m}$
∇T	Temperature Gradient	K / m
σ	Stefan–Boltzmann Constant	$5.67 \cdot 10^{-8} \text{ W} / \text{m}^2 \cdot \text{K}^4$
α	Heat Transfer Coefficient	$\text{W} / \text{m}^2 \cdot \text{K}$
λ	Material's Conductivity	$\text{W} / \text{m} \cdot \text{K}$
ρ	Charge Density	C / m^3

6. References

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