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# Macrorheological Theory of High-Temperature Deformation of Powder Materials under SHS Compaction

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*Abstract*

*The present work surveys the results of mathematical modelling of deformation and thermal processes of SHS compaction of advanced ceramics. Various regimes of SHS compaction have been studied based on a rheodynamic model. The model takes into account the initial density distribution throughout the material and the nonsteady state of the process. The wave regime and the regime having a zone of decreased density in the centre of the specimen are discussed. The influence of delay time on the process of densification is described. It is shown how the model developed facilitates solution of practical problems of that process.* © *1996 Elsevier Science Limited.*

## 1 Introduction

Power SHS compaction is now a most promising and intensively developing SHS variant.[1] It combines combustion and mechanical action upon the heated product, resulting in compact, low-porosity and poreless materials and articles based on simple and complex carbides, silicides, borides, carbonitrides and others, most often with metal bindings and alloying additions. A combination of combustion and high-temperature deformation with application of high pressure to the combustion products is a characteristic feature of all these processes.

The development of various methods of powder SHS compaction has prompted studies of high-temperature deformation of the powders of refractory compounds that are specific rheological objects. These materials are characterised by a high initial porosity (of up to 50%). In a high-temperature (2000–3000 K) region, they behave as highly viscous liquids ($m = 10$ –10 Pa s). Scientifically and technologically, it is important to inves-

tigate the capacity of these materials for compaction. For studying the processes of deformation of powder materials under SHS compaction and analysing nonisothermal flow of compressible media, rheodynamic models are used,[2,3] whose basic parameters are macroscopic density, velocity and stresses in the material. The analysis of the heat and deformation processes is the key to correct understanding of high-temperature compaction and moulding mechanisms in porous materials.

## 2 Theory

As a rule material is pressed in a cylindrical mold, and the equations contained in the statement of the problem will therefore be written henceforth in a system of cylindrical coordinates. It is assumed that flow is unidimensional, with one velocity component $v_z$ (henceforth the subscript z will be omitted) and opposed to the direction of the $z$ axis. With the mentioned assumptions, the problem reduces to the solution of the following system of equations of rheodynamics and heat exchange:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial z}(\rho V) = 0 \tag{1}$$

$$\rho \rho \left( \frac{\partial V}{\partial t} + V \frac{\partial V}{\partial z} \right) = \frac{\partial \sigma_{zz}}{\partial z} \tag{2}$$

$$\sigma_{zz} = (\frac{4}{3}\mu + \xi)\frac{\partial V}{\partial z} \tag{3}$$

$$\sigma_{rr} = \sigma_{\theta\theta} = (-\frac{2}{3}\mu + \xi)\frac{\partial V}{\partial z}, \tag{4}$$

$$c[\frac{\partial(\rho T)}{\partial t} + \frac{\partial(\rho V T)}{\partial z}] = \frac{\partial}{\partial z}[\lambda(\rho)\frac{\partial T}{\partial z}] - \frac{2\alpha}{r_0}(T - T_0) \tag{5}$$

Here it is assumed that the temperature across the section $z$ = const of the pressed compact is constant because its transverse dimension is small in comparison with the length, and that the thermophysical properties of the material do not depend on the temperature. Heat removal in the transverse direction is taken into account by the last term of the equation of heat conduction. We choose the boundary conditions:

$$-\lambda(\rho)\frac{\partial T}{\partial z} = \begin{cases} -\alpha_1(T - T_0), & z = 0, \\ \alpha_2(T - T_0)), & z = z_0, \end{cases}$$

$$\tau|_{z=0} = 0, \quad \sigma_{zz}|_{z=z_0} = -P. \tag{6}$$

The dependence of shear viscosity $\mu$ $(\rho, T)$ and bulk viscosity $\xi$ $(\rho, T)$ on the density and temperature of the compressible material is adopted in the following form:

$$\mu(\rho,T) = \mu_1(T)\mu_2(\rho) = \mu_0 \exp(U/RT)\rho^m,$$

$$\xi(\rho,T) = \frac{4}{3}\mu(\rho,T)\frac{\rho}{1-\rho} = \frac{4}{3}\mu_0 \frac{\rho^{m+1}}{1-\rho} \exp(U/RT). \tag{7}$$

The dependence of viscosities on density is taken from published data[2,3] where the empirical parameter $m$ is chosen on the basis of an experiment.

Here $t$ is time; $r,z$ the transverse and longitudinal coordinates; $T$ the temperature; $r_0$, $z_0$ the radius and height of the compact, respectively; $\rho_1$, $\mu_1$ the density and viscosity of the incompressible base of the material, respectively; $\rho$ the relative density of the material, $\sigma_{zz}$, $\sigma_{\theta\theta}$, $\sigma_{rr}$ the radial, tangential, and axial stresses; $\lambda,c$ the thermal conductivity and specific heat of the material; $\alpha$, $\alpha_1$, $\alpha_2$ the heat transfer coefficients in the transverse direction, at the upper and lower end face of the compact, respectively; $V$ the flow velocity of the material; $P$ the force on the press; $U$ the activation energy of the process; $R$ the universal gas constant.

At the initial instant the distribution of density and temperature in the material is specified:

$$\rho(z,0) = \rho_0(z), \quad T(z,0) = T_*(z) \tag{8}$$

The dependence of thermal conductivity on density is adopted in the form of the power law:[4]

$$\lambda(\rho) = \lambda_0[\rho/\rho_0]^k,$$

where $k$ is an empirical parameter. The movement of the upper boundary of the specimen under the effect of the plunger of the press is taken into account in the model in the following way:

$$V_P = \partial z_0/\partial t.$$

It is pertinent to note that, in solving the system of equations considered, inertial and nonstationary terms in the motion equation are often occasions neglected and these equations are replaced by simpler equilibrium conditions: $\partial\sigma_{zz}/\partial t = 0$. These assumptions are commonly related to the smallness of the Reynolds number for the processes of hot pressing of refractory powdered materials, which is substantiated by evaluations.[5] Strictly speaking, the possibility of disregarding the inertial and nonstationary terms in the equation of motion is determined not only by the smallness of the number Re, but also by the value of partial derivatives of velocity with respect to the coordinates and time. For inertial media the disturbance from the plunger will not propagate throughout the bulk of the material instantaneously, thus creating prerequisites for forming a compaction wave in the porous medium.

## 3 Numerical Results and Discussion

For numerical calculations we go over the Lagrangian mass system of coordinates in which the time $t_L$ is the same as time $t$, and the mass coordinate $q$ has the meaning of relative mass of the material in a volume from 0 to $z$:

$$q = \int_0^z \rho(z,t)dz.$$

For solving the equation of heat conduction (5) together with the boundary (6) and initial (8) conditions we use the method of balance,[6,7] the conservative implicit difference schema, and for solving the finite-difference equations, we use the method of matching and the iteration method.[8,9] Equation (1) is solved by the finite difference method with the use of the implicit four-point difference schema, and eqns (2), (3) and (4) are solved by the finite difference method. As a result of the numerical solution of the problem we find the distribution of temperature, density, velocity, and stresses in the pressed material at any instant.

An analysis of the numerical calculation showed that with nonisothermal pressing the following qualitatively different regimes of compaction are realised: (1) without compaction, (2) maximal compaction, (3) insufficient compaction. The decisive factors in the realisation of a certain regime of pressing are the initial viscosity (at the combustion temperature) and the range within the characteristic temperature interval (from the combustion temperature to the viable temperature). The regime without compaction is realised when the viscosity of the solid base is sufficiently high. In this case there is no noticeable compaction of the material. Figure 1a (curve 1) shows the characteristic shape of the dependence of density on time for $\mu_1 = 10^9$ Pa s. Numerical calculation can establish the critical value of $\mu_*$ above which this regime is
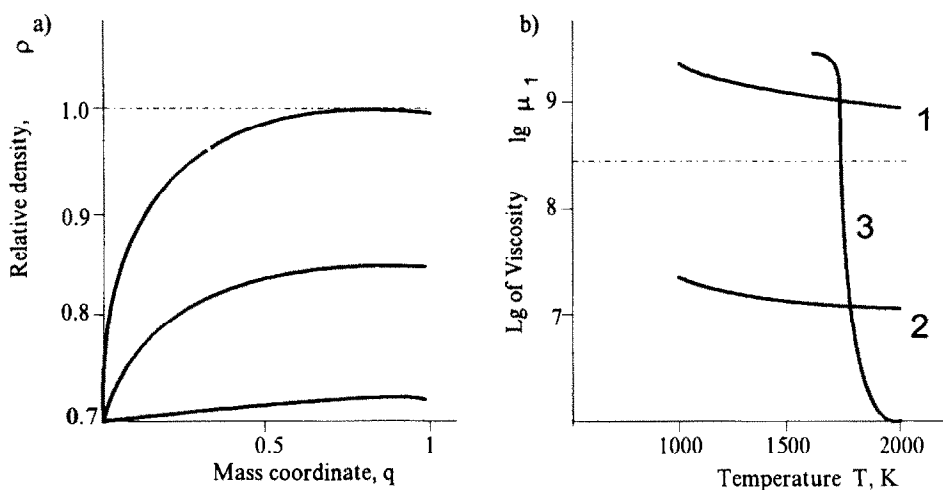
**Fig. 1.** Distribution of density along the mass coordinate $q$ (a) and dependence of the viscosity of the solid phase on temperature (b) for different regimes of compacting material: (1) regime without compaction, (2) regime of maximal compaction, (3) regime of insufficient compaction. Parameters: $P = 10^8$ Pa, $t = 0$ s.

realised. For selected parameters of the problem it was found that $\mu_*$ is equal to $5 \times 10^8$ Pa s (the dashed line in Fig. 1b). If the initial viscosity is higher than the critical one and is a weak function of the temperature (Fig. 1b, curve 1), then $\mu_1(T) > \mu_*$, and the regime without compaction is always realised. A characteristic feature of the regime of maximal compaction is the change of density from the initial value to 1 (curve 2, Fig. 2a). This regime is realised when the initial viscosity of the solid base during the entire process remains lower than the critical one, i.e. $(T) <5 \times 10$ Pa s, as shown in Fig. 1b (curve 2), when a change of temperature entails only a small change of viscosity. If the temperature changes only slightly (coming close to the adiabatic case), compaction proceeds quasi-isothermally, and the process is well described by the isothermal formulas of compaction.[10] However, when the temperature is uniformly distributed throughout the bulk of the material, the model in Ref. 5 can be used. In that case the processes of compaction do not depend on the temperature but the thermal processes depend on density (on account of the dependence of the thermophysical properties on this variable). In the insufficient compaction regime density increases noticeably at the beginning of the process only, when the material still has retained its properties of plastic deformation. Later the material freezes because it is cooled, it loses its viability, and density does not change any more (curve 3 in Fig. 1a). This regime is realised when the initial value of viscosity of the incompressible base is lower than the critical $\mu$ but higher in the course of the process than the critical value in consequence of the strong dependence on the temperature (curve 3 in Fig. 1b). Under the conditions of this regime the thermal processes and processes of com-

paction proceed correlatively. Thus, variation in the temperature dependence of the viscosity of the solid base alone ensures a continuous transition from one regime of compaction to another.

Figure 2 shows the dependence of the density and temperature on the height of the material at a different point in time. At the initial point in time the bottom is denser than the top. For this type of initial density distribution, we have a zone of decreased density in the centre of the specimen. Such an effect was observed under SHS compaction of carbides in Ref. 11. The results obtained by us show that it can be due to the nonsteady state of the process.

The results of the numerical experiment show that under SHS compaction the wave regime of compaction of the hot porous mass takes place. As a criterion determining the presence of one or other compaction regime we choose the relationship
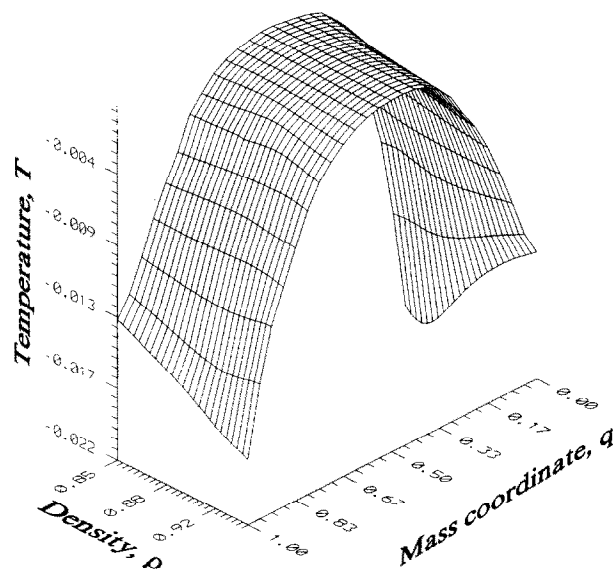


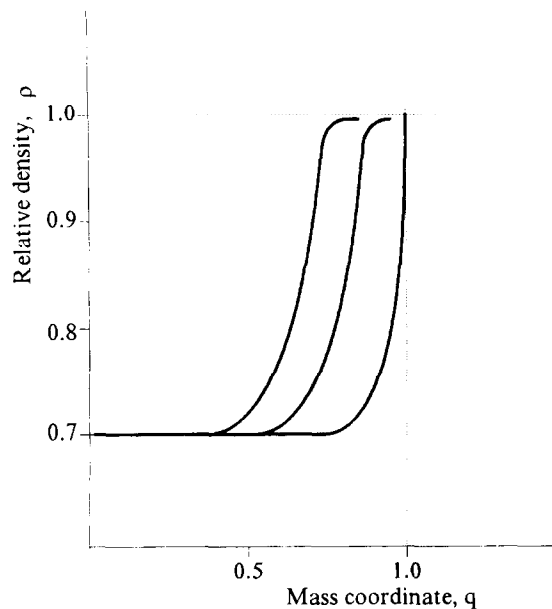**Fig. 2.** Dependence of the density ($\rho$) and temperature ($T$) on the mass coordinate ($q$).

**Fig. 3.** Density distribution with the mass coordinate of the compact for the wave regime of the compaction.



**Fig. 4.** Distribution over the specimen in dependence on the delay time (a) of relative density, (b) of the radial stresses: 1-delay time = 0, 2-delay time = 5 s, 3-delay time = 10 s. Parameters: $P = 10^8$ Pa, $\mu_1 = 10^7$ Pa s.

among compaction time, the time of thermal relaxation and hydrodynamic relaxation. Such a regime can be realised (Fig. 3), for example, under conditions where the time of hydrodynamic relaxation is more than the compaction one.

The present model made it possible to investigate the effect of the delay time on the distribution of density and of stresses in the material (in accord with the statement of the problem, the axial stresses $\sigma_{zz}$ are constant, and the tangential stresses are equal to the radial ones $\sigma_{\theta\theta} = \sigma_{rr}$, henceforth we will therefore confine ourselves to dealing with the radial stresses $\sigma_{rr}$). With short delay times and uniform initial temperature distribution (T = 2000 K), a uniform state of stress is attained in the material within the characteristic time of compaction (Fig. 4a, curve 1), and the compressive stresses are maximal (Fig. 4b, curve 1), which is a sign of good quality of the finished product. When the delay time is longer, the gradient of radial stresses over the specimen increases in consequence of strong cooling of the material from the end faces, an ever-increasing part of the material near its end faces remains incompletely compacted (Fig. 4a,b curves 2,3), and the maximal density of the material also becomes substantially lower.

## 4 Conclusion

The model under consideration makes it possible to calculate the technological regimes of compacting SHS materials and to predict the quality of products from the point of view of the level of thermal gradients as well as of the state of stress
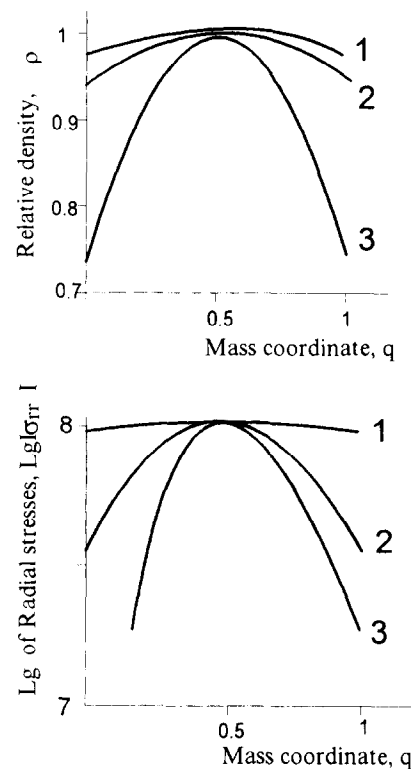
of the material and of the density distribution. It is assumed that on its basis the process of SHS pressing can then be optimized.

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