Modeling the Structure and Processes of Heat Transfer in Beds of Aluminum Micro- and Nanopowders

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Abstract. A model of the structure and a method for calculating (forecasting) the thermal conductivity of beds from coarse to nano-dispersed aluminum powders are developed. A significant change in the thermal conductivity of the particles themselves was taken into account during the transition from the micro-meter to the nanometer-sized range of particle sizes. The thermal conductivity was calculated over a wide range of particle sizes, granular structure skeleton porosity, and total porosity of the beds.

1. Introduction
The desire to minimize the operations of forming metal parts, reduce energy costs, time and temperature of sintering parts led to the development of powder metallurgy. The process of manufacturing parts consists of two stages - pressing the powder and subsequent sintering, the temperature and duration of which significantly decrease with a decrease in the particle size of the powders and the primary porosity of the compacts. Optimization of the technological modes of sintering requires knowledge of the thermal properties of sintered powders, their heat capacity and thermal conductivity. But a decrease in the particle size leads to a change in the structure of the bed (see figure 1) and a decrease in the thermal conductivity of the powders, usually by one and a half to two orders of magnitude compared to the thermal conductivity of the monolithic metal, which increases the sintering time.

2. Structure model and the method for calculating thermal conductivity
The structure of the beds of powder materials observed using a stereomicroscope is shown in figure 1. In powders of the micrometer range with a particle size of 1<\textless d <100 \textmu m, the main decrease in the thermal conductivity of the powders occurs due to an increase in the porosity of the beds and a decrease in the thermal conductivity of the gas located in small gaps between the contacting particles (the Smoluchowski-Knudsen effect), when the distances between the surfaces of the contacting particles become less than the mean free path of gas molecules.
In the sub-micron nano-range of 10<d<1000 nm particle sizes, along with a decrease of the thermal conductivity of the gas located between the particles, there is a decrease in the thermal conductivity of the metal particles themselves, when the mean free path of heat carriers (electrons, phonons) becomes comparable [2] with the size of ultrafine spherical particles.

![Figure 1. The structure of powder beds: (a) beds of large particles 0.5 mm<d<5 cm, porosity P of the bed 0.3<P<0.5; (b) beds of micro- and nano-dispersed particles with high porosity 0.75<P<0.95; 1-frame "bars" with contacting particles, 2-"large pores" between the frame bars [1].](image)

A polystructural modification of the model (see figure 2) of beds of macro-, micro- and nano-dispersed powders and a method for calculating their effective thermal conductivity, taking into account the change in the thermal conductivity of gas and solid particles in a wide range of the powders particle size, are proposed. The structure of the bed is formed by a frame with a relatively dense packing of contacting particles and larger pores penetrating the frame bars.

![Figure 2. The polystructural model of powder bed.](image)

The calculation of thermal conductivity of the powder bed is carried out in two stages. At the first stage, the thermal conductivity \( \lambda_k \) of the frame bars formed by continuously contacting spherical (sp) particles is determined. The porosity of the frame \( P_k \) varies within 0.26<P_k<0.4.

The thermal conductivity of the frame \( \lambda_k \) is calculated [1] by the formulas:

\[
\lambda_k = \frac{\lambda_{sp}}{y_3^2} \left[ \frac{D}{y_3^2} + \lambda_{T4} \left( D - 1 - \omega \ln \frac{\omega - D}{\omega - 1} \right) \right]^{-1} + \lambda_{T4} (y_3^2 - y_3^4),
\]

\[
\lambda_{sp,3} = \lambda_{sp,3,mol} + \lambda_{sp,3,rad} = \frac{\lambda_{g(H_0)}}{14B/(H\Delta_{sp,3})} + 4\varepsilon_\text{fr} \sigma_{S-B} T^3 \Delta_{sp,3},
\]

where: \( \lambda_{sp} = f(d) \) - thermal conductivity of aluminum particles of different sizes; \( \lambda_{sp,3} \) - thermal conductivity of the medium in the gap between the contacting particles; \( \Delta_{sp,3} \) - average integral thickness of the spherical gap between the contacting particles [1]. \( N_k(P_k) \) is the average number of contacts per each particle of the frame, depending on the porosity of the frame \( P_k \).

\[
N_k(P_k) = \{ P_k + 3 + [(P_k)^2 - 10P_k + 9]^{0.5} \} / (2P_k),
\]
The results of calculations of the effective thermal conductivity of beds of micro- and nano-dispersed aluminum powders are shown in Fig. 3. They are presented in a semilogarithmic form, which is due to the second stage of the calculation, the structure of the bed of microspheres as a whole is determined by the sum of the molecular $\lambda_{\text{mol}}$ and radiant $\lambda_{\text{rad}}$ components:

$$\lambda_{\text{sk}.p.2} = \lambda_{\text{sk}.p.2} \text{ mol} + \lambda_{\text{sk}.p.2} \text{ rad}.$$  

The contribution of the thermal energy transfer $\lambda_{\text{sk}.p.2} \text{ mol}$ is determined by the expression

$$\lambda_{\text{sk}.p.2} \text{ mol} \approx \frac{\lambda_2(H_0)}{1+t/(H_{1.p} P_3)}.$$  

If there are experimental data on the value of the thermal radiation attenuation coefficient $\alpha_{\text{att}}$ (m$^{-1}$), then the contribution to the thermal conductivity of through pores forming a second order structure with the frame [1] from the transfer of thermal energy by radiation $\lambda_{\text{sk}.p.2} \text{ rad}$ is defined by the expression

$$\lambda_{\text{sk}.p.2} \text{ rad} \approx 0.3 \left( \frac{T}{1000} \right)^{3/4} \frac{1}{\alpha_{\text{att}}}.$$  

In the absence of experimental data, the contribution of thermal energy transfer in the through pores of the second-order structure $\lambda_{\text{sk}.p.2} \text{ rad}$ is estimated by the formula

$$\lambda_{\text{sk}.p.2} \text{ rad} = 4 \epsilon_{\text{pr}} \sigma_{\text{S- B}} T^3 L_{p.2}.$$  

3. Results and discussion

The results of calculations of the effective thermal conductivity of beds of micro- and nano-dispersed aluminum powders are shown in Fig. 3. They are presented in a semilogarithmic form, which is due to

$$B = \frac{4\gamma}{\gamma + 1} \frac{2-a}{a} L_{\text{fr.p.}} H_0 \text{Pr}^{-1},$$

here: $\gamma = c_p/c_v$ - adiabatic exponent; $c_p$, $c_v$ - isobaric and isochoric heat capacity of the gas located between the bed particles; $a$ is the coefficient of accommodation of gas molecules filling particle pores. For air $a \approx 0.97$; Pr - Prandtl number (criterion), for air it is 0.7; $L_{fr.p.}$ - mean free path of gas molecules in pores at atmospheric pressure $H_0 = 760$ mm Hg.
the scale of the range of particle size variation by more than 4 orders of magnitude. A significant decrease in the average particle size is accompanied by a decrease in the thermal conductivity of aluminum particles from 200 to 65 W m\(^{-1}\) K\(^{-1}\) [2], as well as in the size of the gas interlayer between the particles and the thermal conductivity of the gas from 2.6*10\(^{-3}\) to 2.5*10\(^{-3}\) W m\(^{-1}\) K\(^{-1}\) in large pores between the frame bars and up to 2.8*10\(^{-4}\) between the small particles of the frame. The effective thermal conductivity of beds of large (by the scale of powder metallurgy) and highly heat-conducting aluminum particles monotonously decreases more than 3 times from 0.75 to 0.2 W m\(^{-1}\) K\(^{-1}\) with increasing porosity up to P = 0.85, which is confirmed by a lot of experimental data. A slight increase in the effective thermal conductivity at a porosity of P > 0.85 is due to an increase in the contribution of radiation in large through pores between the frame bars.

4. Conclusion
The listed processes lead to anomalous character of the dependence of the effective thermal conductivity of beds on porosity and large-scale decrease in the thermal conductivity of low-porous beds by more than 3 orders of magnitude shown in figure 3. The proposed structure model and the method for calculating thermal conductivity of beds of aluminum powders in the micro- and nano-size ranges can be used to predict the thermal conductivity of the beds even at the initial stage of the development of powder composites, before the availability of reliable experimental data.

Figure 3. The scale of changes in the effective thermal conductivity of beds of micro- and nano-dispersed aluminum particles \(\lambda_{\text{eff}} = f(\lambda_{\text{sp}}(d), \lambda_g, d, P_k, P)\).

5. References
[1] Dul'nev G N and Zarichnyak Yu P 1974 Thermal Conductivity of Mixtures and Composite Material (Leningrad: Energiya) p 264
[2] Huang Cong-Liang et al. 2013 Thermal conductivity of metallic nanoparticles Acta Physica Sinica 62(2)