Meso-porous Modeling for Theoretical Analysis of Sinter Ores by the Phase-field, Unit-cell Method

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A high-graded sinter ore has meso-pores to have large surface area and fine channel structure enough to enhance gas reduction reaction. In the conventional processing, macro pores are inevitably generated together with these meso-pores, resulting in significant reduction of stiffness and strength of sinter ores. Hence, there have been very few reports on the optimal design of meso-porous solid structure toward an ideal sinter ore which has a sufficient amount of meso-pores for low temperature reduction and has a sufficient level of mechanical strength and thermal conductivity. Multi-level modeling with use of artificial unit cells is proposed to aim at the meso-porous microstructure design. The phase filed method with finite element modeling provides us a reliable tool to control the size, shape and distribution of meso-pores and to consider their effects on the mechanical and thermal properties of sinter ores. Meso-porous hematite is employed as a targeting sinter ore to describe actual meso-porous microstructure by comparing the experimentally measured Young’s moduli with the theoretically predicted elastic properties. Microstructure with uniform distribution of isolated meso-pores provides the upper bound on the Young’s modulus. Reduction of Young’s moduli in experiments below this upper bound is caused by irregular shaping and coalescence of meso-pores during sintering. Unit-cell modeling with irregularly shaped and inter-connected meso-pores, provides an actual upper bound for measured elastic properties of sinter ores. Variation of thermal conductivity with the average porosity is also estimated as a master curve for optimum sintering process design.

KEY WORDS: sinter ore; meso-porous unit cell; phase field method; theoretical model; elastic properties; thermal conductivity.

1. Introduction

A high-graded sinter ore has meso-pores to have large surface area and fine channel structure enough to enhance gas reduction reaction. In the conventional processing, macro pores are inevitably generated together with these meso-pores, resulting in significant reduction of stiffness and strength of sinter ores. Hence, there have been very few reports on the optimal design of meso-porous solid structure toward an ideal sinter ore which has a sufficient amount of meso-pores for low temperature reduction and has a sufficient level of mechanical strength and thermal conductivity. This is partially because reduction of stiffness and strength with increasing the porosity has become a common sense and no further works are believed to be necessary for design of meso-pores. Mechanical treatise on the equivalent inclusion in the elastic continuum suggests that pore shape and its distribution should have significant influence on the relationship between the elastic properties and the average porosity. In the conventional theory for an actual porous medium, the elasto-plastic treatise is applied to formulation of finite element analysis for sintered materials by modifying their constitutive equations. Only the average porosity is taken into account of these methods to consider the effect of pores on its mechanical behavior. In the actual porous materials, various types of pores are distributed in the matrix. Macro-pores or cavities with the size of millimeters coexist together with meso-pores in the micrometer range and micro-pores in the sub-micrometer range. In order to discuss the effect of meso-pore size and geometric distributions on the mechanical response of meso-porous medium, a new reliable method is necessary.

Authors have proposed the multilevel modeling for sintering and hot deformation and the multi-scale analysis for creep damage and fracture. In these methods, a unit cell model is used to describe the microscopic evolution and to quantitatively estimate the mechanical properties. Since a macro-model is combined with this unit cell model, macroscopic response of a whole sinter-ore specimen is also analyzed in the similar manner to microscopic analysis by the unit-cell modeling. Furthermore, a real microstructure of polycrystalline materials and sinter-ores is considered in this unit-cell model to make strength and stiffness analyses of these materials in practice. Although a representative volume element for actual sinter-ore texture can be built in by this real microstructure modeling, mechanical understanding on the texture and meso-pores is limited by experimental observation since the unit-cell models are only made from the observed micrographs. A new theoretical method is further needed to consider a wide variety of meso-pore shapes and distributions into a unit-cell modeling for total description of mechanical behavior in the...
porous microstructure of sinter-ores.

In the present paper, an artificial cellular material modeling\textsuperscript{10,11} is applied to make a meso-porous material design by unit-cell modeling. The phase field method (PFM) is first used to generate various geometric configuration of meso-porous microstructure. A physical process to actually form pores or foams in practice is modeled by using PFM. Variety of meso-porous microstructure models is generated by the nucleation, coalescence and growth processes of meso-pores. Implementation of mechanical compatibility is taken into account to transform the generated microstructure model to a mathematical model by the finite element method. Meso-porous hematite is taken for a material to discuss the effect of meso-pore size, shape and distribution on the mechanical properties. Uniform distribution of the isolated meso-pores provides the upper bound instead of the conventional volume averaging. It is theoretically proven that actual Young’s modulus of sinter ores is reduced by the irregular shape and distribution of meso-pores in their microstructure. Unit-cell modeling with consideration of irregular-shaped and inter-connected meso-pores provides an actual upper bound of experimental elastic properties. Effect of meso-pores on the thermal conductivity is also quantitatively evaluated by the present method.

2. Artificial Unit-cell Modeling for Sinter-ore

In the multi-level modeling for sinter ores, their local part is composed of a unit cell, which represents their characteristic microstructure. There are two methods to construct this unit model: real microstructure modeling and artificial unit-cell modeling. In the former, optical micrograph, SEM (Scanning Electron Microscopy) and TEM (Transmission Electron Microscopy) micrographs are used to extract an objective unit cell, which is free from geometrical dimension.\textsuperscript{8,9} Although this method enables us to generate a unit-cell model on the basis of real texture and its composites, parametric survey with wide variety of textures or virtual design of fine porous media are impossible to consider. In the latter, a unit cell is artificially designed on the basis of computational geometry or microstructure evolution kinematics. Although the generated unit cell does not always correspond to real microstructure, effect of porosity or fine pore distribution in sinter ores on the mechanical properties is directly taken into account of materials and processing design.\textsuperscript{12}

Figure 1 depicts a multi-level modeling for sinter ores with use of artificial unit cell modeling. Mechanical response of macro-pores or cavities in the ore is considered by the macro-model in the multi-level modeling. The unit cell takes meso-pore distribution into account, so that equivalent elastic moduli as well as thermal conductivity are theoretically estimated together with stress and thermal analyses for the whole sinter ore. Typical two and three dimensional unit-cell models, which are artificially generated, are shown in Fig. 2. Depending on the average porosity, nucleated meso-pores recombine and redistribute to form a characteristic porous configuration as a unit cell.

To be explained later, nucleation and kinematical development of meso-pores must be rationally designed in the present method. This approach is based on the phase field method (PFM), which has been successfully applied to nucleation and growth of polycrystalline materials.\textsuperscript{10} In general, a targeting microstructure is represented by a set of orientation variables, \( \eta_i(r) \), \( \eta_j(r) \), ..., \( \eta_k(r) \). Each region is exclusively distinguished by this \( \eta_i(r) \): e.g. its absolute value becomes unity for the \( i \)-th region and \( \eta_j(r) \)’s for \( j \neq i \) are zero. Due to Cahn’s and Hilliard’s treatment, the free energy functional to be minimized is obtained for this inhomogeneous system.\textsuperscript{13}

In the present meso-porous modeling, one orientation variable is employed to represent dense, solid texture by \( \eta=0 \) and the vacant medium, by \( \eta=1 \), respectively. When starting from the nucleation sites of pores, each pore grows in the shape of concentric circle, combines with other pores and coarsens with time. Figure 3 depicts the nucleation and growth of meso-pores which are calculated by the present method. Although geometric configuration is generated for meso-porous materials, their mechanical and thermal analyses are impossible from as-generated models in Fig. 3. In order to generate a meso-porous unit-cell model, its theoretical procedure must be built in by combining the PFM driving process with the implementation of finite elements.

![Fig. 1. Multi-level modeling with use of meso-porous unit cell for stiffness/strength and thermal analyses of sinter ores.](image1)

![Fig. 2. Two and three dimensional representative unit cell models with meso-pore distributions: (a) two dimensional model, (b) three dimensional model, and (c) meso-pore linkage in the three dimensional unit-cell model.](image2)
3. Theoretical Procedure to Generate Meso-porous Unit-cell Models

The present procedure is mainly divided into four processes to generate a meso-porous unit-cell model.

3.1. Nucleation Process of Meso-pores

Nuclei of meso-pores are distributed in the unit-cell domain with statistical randomness. Since the present model is formulated and discretized by the finite difference method (FDM), the initial nuclei of meso-pores are sited at the selected nodes in FDM. The meso-pore is controlled to grow from this pointwise nuclei and to have the prescribed pore size and shape.

With consideration of subsequent coalescence and growth processes, the inter-nuclei distance becomes a key to control the size, shape and their distribution. If the nuclei are distributed to be completely isolated from each other, meso-pores are aligned uniformly in the unit-cell domain, as shown in Fig. 4. A unit cell with regularly aligned meso-pores is thought to be elastically equivalent to a perforated medium, which was analyzed by the conventional micromechanics. In this ideal case, the generated meso-pores have less or no mechanical interactions among them. Since the averaged stress is enhanced only by local strain concentration at the vicinity of a single meso-pore, reduction of elastic moduli from that of the fully dense matrix is minimized. That is, this modulus is thought to be an upper bound of the elastic moduli calculated for the variety of meso-porous media.

3.2. Growth Process of Meso-pores

In the actual sintering process, meso-pores are governed by its growth to larger pores and its coalescence with other pores. Other parameters than the average porosity have never been considered in the conventional approaches to describe the mechanical properties of sintered materials. Geometrical coalescence and growth of meso-pores are taken into account of the present method. At first, inter-nuclei distance is predetermined to allow each pore to have interaction as the initial set-up. Each meso-pore grows by itself to minimize the total free energy function. During this temporal growth of pores, some meso-pores are forced to be combined to make an irregularly shaped pore. Figure 5 depicts a typical coalescence and growth behavior of meso-pores.

3.3. Implementation of Kinematic Compatibility

Although geometries of meso-pores are obtained by using the phase filed method, both displacements and strains are difficult to be defined across the boundaries. Since they have finite width between adjacent two regions, continuity of displacement as well as compatibility of strains are impossible to be implemented on these diffuse boundaries. In order to build up the rational mathematical models for mechanical analysis, each boundary with diffuse width must be translated to an inter-cell edge, which is co-shared with adjacent cells in the two dimensional modeling. In the three dimensional situation, it must be translated to an inter-cell plane with inter-cell edges. In the present method, a color segmentation algorithm is applied to define the locations of inter-cell boundary for each cell. These locations are archived to redefine the inter-cell boundary as a closed loop. In this two-dimensional geometric model, each cell domain is uniquely defined as a polygonal tessellation and isolated from each other by a continuous connection of cell walls or matrix, as shown in Fig. 6.

3.4. Automatic Generation of Mathematical Models

In the following simulations, the finite element method is
employed as a mathematical formulation for the present unit-cell modeling. Hence, the solid fraction of a unit cell having meso-pores must be accurately subdivided to an assembly of elements without overlapping and penetration of elements. In addition, each finite element is connected at nodal points in order that displacement should be continuous across each inter-element edge. Figure 7 depicts a typical procedure to transform the geometric data of a unit-cell model to the mathematical model with finite elements and nodes. A set of geometric models and finite element information is used for mechanical and thermal analyses by the unit-cell modeling. In the following analyses, the piecewise displacement in each finite element is approximated by complete linear function. When using this type of simple triangular element, several element layers are necessary to have the numerical errors within the tolerance.

4. Theoretical Analysis of Meso-porous Hematite

Meso-porous hematite is employed as a typical sinter ore to describe the effect of porosity size, shape and their distribution on its elastic and thermal properties.

4.1. Rational Generation of Meso-porous Unit Cells

The first rational method to generate the meso-porous unit cells is a nucleation process of cell elements in the unit-cell region. With the prescribed porosity of $\alpha$ and average pore size, the number of meso-pore nuclei is determined. Through the random distribution of these nuclei in the inside of the unit-cell, a meso-porous unit-cell model is generated. By using the present procedure without the growth model, a mathematical model is constructed from each meso-porous unit cell with the prescribed average porosity. Figure 8 depicts the variation of meso-porous unit-cell models with increasing the average of porosity from $\alpha=0.05$ to $\alpha=0.2$. Since the nucleation sites are generated to satisfy the isolation condition, each meso-pore in Fig. 8 distributes with the specified distance from its neighboring pores.

Among various characterizing parameters of meso-pores, the specific surface area ($S$) was calculated from the unit cells in Fig. 8. In general, when the isolated pores have a constant pore size ($d$), the specific surface density as well as the average porosity, are given by

$$
S = n \times (\pi d) \quad \text{and} \quad \alpha = n \times (\pi d^2/4) \quad \ldots \ldots \ldots \ldots \quad (1)
$$

where $n$ is the meso-pore density in the unit cell, which is only a variable both in $S$ and $\alpha$. Hence, $S$ is proportional to $\alpha$: $S=(4/d)\alpha$.

Figure 9 shows the normalized specific surface area ($S_n$) versus the average porosity. Here, $S_n(\alpha)$ is defined by $S(\alpha)/S_1(0.05)$ where $S_1(0.05)$ is the specific surface area calculated for the unit cell, Fig. 8(a) when $\alpha=0.05$. The whole $S(\alpha)$'s are calculated for all the unit cells in Fig. 8. As theo-
and coalescence of meso-pores, with the porosity for various porous configurations. Due to growth processes, the unit cells with smaller isolated pores since the nucleation sites are nearly the same between two. Coalescence and growth processes are taken into account for the unit cells in Figs. 8(a) to 8(h). In Fig. 8, the unit cells from Figs. 8(e) to 8(h) have a half pore size of unit cells in Figs. 8(a) to 8(d); then, theoretically, $S/\alpha$ for unit cells with larger pores must become a half of $S/\alpha$ for those with smaller pores. Corresponding to this theoretical estimate, $S/\alpha=38.6\pm1.7$ for the unit cells in Figs. 8(e) to 8(h) and $S/\alpha=20.5\pm0.5$ for the unit cells in Figs. 8(a) to 8(d).

4.2. Controllability of Meso-porous Configuration

Coalescence and growth processes are taken into account of model construction to control the meso-porous configuration. Figure 10 depicts two types of configurations with $\alpha$ nearly equal to 0.2. Complex shaped or connected pores are generated together with isolated meso-pores. In the conventional theoretical treatment, the porous medium is assumed to be a continuum with the specified porosity of $\alpha$. In the present modeling, various unit-cell configurations are utilized to consider the effect of porosity shape and its distribution on the mechanical response even when the average porosity is nearly constant. $S-\alpha$ relationship is also calculated by using the unit cells in Fig. 10 and shown again in Fig. 9. For $\alpha<0.05$, $S_0$ becomes nearly the same as $S_n$ for the unit cells with smaller isolated pores since the nucleation sites are nearly the same between two. Due to growth and coalescence of meso-pores, $S_0/\alpha$ decreases monotonically with $\alpha$.

Pore size distribution is also an important parameter to characterize the meso-pore shape distribution in ores. The homogenized Young’s modulus $E$ is defined by using $D_{ijkl}$.

$D_{ijkl} = \frac{1}{V} \int \left( D_{ijkl} - D_{ipjq} \frac{\partial \chi_p}{\partial q} \right) dy$ \hspace{1cm} (2)

where $D_{ijkl}$ is the elastic modulus tensor of dense materials, $\chi_p$ the characteristic function, $v_i$ the local coordinates of a unit cell, and $V$ the unit cell volume. In the formulation of Eq. (2), the summation index rule is used for simplicity.$^{16}$ The homogenized Young’s modulus $E$ is defined by using $D_{ijkl}$.

Reference 14) experimentally discussed the effect of powder shape irregularity on the powder size distribution. If the above discussion is true to the relationship between pore shape and pore size distributions, the averaged pore size becomes larger with increasing the porosity. Figure 11 depicts the cumulative population of pores in the function of normalized pore size $D_n$ for unit cells with different porosity. $D_n$ for an irregularly shaped pore is defined by the ratio of the diameter of its circumscribing circle to the unit length. The averaged pore size at 50% of cumulative population increases with the porosity. This qualitative agreement with experimental characterization assures that pore shape irregularity should be evaluated by the present method.

4.3. Elastic Response of Meso-porous Hematite

Effect of the porosity on the elastic modulus for the sinter ores has been experimentally discussed in literature.$^{15}$ Unfortunately, testpieces of sinter ores have various kinds of meso-pores in them even when they have the same averaged porosity. The fluctuation in the measured elastic moduli experimentally measured, often comes from the difference in meso-porous configuration in microstructure. Since various meso-porous configurations are considered in the present method, the effect of meso-porosity size, shape and their distribution on the elastic moduli is directly considered.

Meso-porous hematite is employed for simulation. In the actual computation, fully dense hematite material is assumed to have the Young’s modulus of 200 GPa (or $E_0=200$ GPa) and the Poisson’s ratio of 0.3.$^{15}$ For simplicity of theoretical modeling, the meso-pores are represented to be an elastic medium with the reduced Young’s modulus by $E_0/1000$. The homogenized stiffness tensor $D_{ijkl}^H$ is calculated by the following equation:

$$D_{ijkl}^H = \frac{1}{V} \int \left( D_{ijkl} - D_{ipjq} \frac{\partial \chi_p}{\partial q} \right) dy$$ \hspace{1cm} (2)
These Young’s moduli are further normalized by $E_1^N = E_1/E_0$ and $E_2^N = E_2/E_0$, where $E_0$ is the Young’s modulus for fully solid hematite. Figure 12 depicts the variation of normalized Young’s modulus $E^N$ with increasing the porosity of $\alpha$. The solid square and triangle symbols represent the calculated $E^N = ([E_1^N + E_2^N]/2)$ using the unit-cell models with uniformly distributed meso-pores, (a) to (d) and (e) to (h) in Fig. 8, respectively. The solid line denotes the volume averaged $E^N$ in geometry. The volume averaged $E^N$ is always much larger than the present solutions in Fig. 12 since no local strain concentration is taken into account. This implies that the conventional estimate has intrinsic risk of overestimation for elastic moduli of porous media. Even when using two meso-porous models with a uniform distribution for different pore sizes in Fig. 8, the calculated $E^N$ is nearly the same between two. Size of meso-pores has nothing to do with the elastic properties as suggested from the theoretical treatise. This agreement of calculated normalized Young’s modulus between two discretized models, assures that the present mathematical model has sufficient accuracy even for stress and strain analysis. Hence, $E^N-\alpha$ relationship is strongly affected by meso-pore shape and its distribution. The calculated Young’s moduli by the unit-cell model with irregularly shaped meso-pores, are compared in Fig. 12 with other data. Irregularity of meso-pore shapes leads to significant reduction of elastic properties. Hence, actually measured elastic properties are estimated theoretically as an upper bound by using the adequate unit cell models with consideration of irregularly shaped meso-pores.

The experimentally measured data are also compared with the calculated $E^N$. For $\alpha<0.05$, the theoretical prediction by assuming the uniform distribution of meso-pores provides an upper bound of measured Young’s moduli for porous hematite. This is because most of meso-pores are isolated in the low-porosity hematite. Table 1 lists both the experimentally measured and present theoretical results when $\alpha$ is nearly equal to 0.05 and 0.10. Even when $\alpha>0.05$, the theoretical $E^N$ by assuming irregularly-shaped meso-pores, is much smaller than those by isolated meso-pores. They become an actual upper bound of experimental results. This reveals that meso-porous hematite is mechanically equivalent to a unit-cell model with the inter-connected and irregularly shaped meso-pores. This reduction of equivalent Young’s modulus comes from the stress or strain concentration at the local region around the actual meso-pores in microstructure in addition to the three dimensional effect on the experimentally measured elastic modulus.

In order to investigate the decrease of elastic modulus by irregularity of porosity shape and coalescence of meso-pores in microstructure, stress distribution in the meso-porous medium was calculated by using the present unit-cell modeling. Fig. 13(a). In the present methods, stress ($\sigma_{ij}$), strain ($e_{ij}$) and displacement ($u_i$) distributions in the unit cell are defined by

Table 1. Comparison of the normalized Young’s modulus between theoretical prediction by the unit-cell modeling and experimental results when $\alpha$ is nearly equal to 0.05 and 0.1.

<table>
<thead>
<tr>
<th></th>
<th>$\alpha = 0.05$</th>
<th>$\alpha = 0.10$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volumetric average</td>
<td>0.95</td>
<td>0.90</td>
</tr>
<tr>
<td>Isolated meso-pore</td>
<td>0.86</td>
<td>0.75</td>
</tr>
<tr>
<td>Complex-shaped meso-pore</td>
<td>0.83</td>
<td>0.65</td>
</tr>
<tr>
<td>Experiments</td>
<td>0.80</td>
<td>0.60</td>
</tr>
</tbody>
</table>

Fig. 12. Variation of the calculated Young’s modulus with increasing the average porosity for meso-porous hematite with comparison of experimental results.

Fig. 13. Stress analysis of meso-porous microstructure by using the present unit-cell modeling: (a) mathematical model for strength and stiffness analyses, and (b) equivalent stress distribution in the meso-porous unit cell.
\[
\sigma_{ij} = D_{ijkl}(\varepsilon_{kl} - \varepsilon_{kl}^0) \quad \text{..........................(4)}
\]
\[
\varepsilon_{ij} = \frac{1}{2}(u_{ij} + u_{ji}) \quad \text{..........................(5)}
\]
\[
u_i = \nu_i^0 + \varepsilon_i \quad \text{..........................(6)}
\]

where \( \varepsilon_{kl}^0 \) is the residual strain distribution in the unit cell, \( \varepsilon \), the periodicity, and \( \{u_{ij}, \nu_i\} \) denotes a pair of displacement in the macro model and the unit cell, respectively.

In this computation, the macro model is subjected to uniform strain state with \( \varepsilon_{kl}^0 = 0; \) e.g. \( \varepsilon_{11}^0 \) is a uniform compressive strain and other strain components are zero. Then, actual stress state is calculated by Eqs. (4)–(6). As depicted in Fig. 13(b), noticeable stress concentration is observed at the vicinity of irregularly shaped pores and between neighboring irregular meso-pores. This local stress concentration leads to significant reduction of elastic modulus.

4.4. Thermal Conductivity of Meso-porous Hematite

Thermal conductivity is generally thought to be also sensitive to porosity than the elastic modulus. Unit-cell modeling is also effective to estimate the homogenized thermal conductivity in the similar manner to estimate of the homogenized elastic stiffness tensor. That is, the homogenized thermal conductivity tensor \( \kappa_{ij} \) is given by

\[
\kappa_{ij} = \frac{1}{V} \int \left( \kappa_{ij}^0 - \kappa_{ij}^0 \frac{\partial \nu_i}{\partial y_j} \right) dy \quad \text{..................(7)}
\]

where \( \kappa_{ij}^0 \) is the thermal conductivity of fully dense hematite. From this \( \kappa_{ij}^0 \), the normalized thermal conductivities \( \kappa_{ij}^N \) and \( \kappa_{ij}^C \) are defined by

\[
\kappa_{ij}^N = \left[ \kappa_{ij}^0 - \left( \kappa_{ij}^0 \right)^2 / \kappa_{ij}^0 \right] / \kappa_0 \quad \text{..........................(8-1)}
\]
\[
\kappa_{ij}^C = \left[ \kappa_{ij}^0 - \left( \kappa_{ij}^0 \right)^2 / \kappa_{ij}^0 \right] / \kappa_0 \quad \text{..........................(8-2)}
\]

where \( \kappa_0 \) is the thermal conductivity of fully dense hematite. Then, \( \kappa^N = (\kappa_{ij}^N + \kappa_{ij}^C)/2 \).

Figure 14 depicts the variation of \( \kappa^N \) with increasing the average porosity for porous hematite. In the similar manner to prediction of elastic properties, irregularity in meso-pore shapes and its distribution has significant influence on the reduction of thermal conductivity with increasing the average porosity. Effect of pore shape distribution on the anisotropy of thermal conductivity is also evaluated by this method.

5. Conclusion

In the sintering process of ores, various kinds of pores are inevitably generated and formed. Among them, meso-pores have significant influence on the mechanical properties. Their size, shape and distribution are thought to be a main factor to determine the mechanical properties of sinter ore. A new unit-cell model is proposed on the basis of the phase field method (PFM) and the finite element method (FEM). Using PFM, the nucleation, coalescence and growth processes of meso-pores are directly considered so that variety of meso-porous configurations is generated as a unit cell model. Through implementation of kinematic compatibility across the boundaries, the above meso-porous unit-cell model is translated to the mathematical model for mechanical analyses. Meso-porous hematite is employed as a targeting sinter ore to demonstrate that Young’s modulus as well as thermal conductivity of meso-porous sinter ores can be theoretically predicted by the present method. With consideration of irregularly shaped meso-pore distribution, theoretical estimate becomes an actual upper bound limit of experimentally measured elastic properties. Various types of meso-porous configuration are taken into account of this method. On the basis of the relationship between meso-porous microstructure of sinter ores and their mechanical properties, an adequate microstructure of ores can be rationally designed to have as-demanded elastic properties or thermal conductivities.

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