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Theoretical and Lattice Monte Carlo analyses on thermal conduction in cellular metals

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Abstract This work addresses the effective thermal conductivity of cellular metals. Analytical relations for upper and lower bounds are evaluated. Formulae for effective conductivities are developed for an accurate estimation. In addition, extensive thermal Lattice Monte Carlo analyses are performed on a range of geometries. Next to simplified model structures, real geometries are addressed that exhibit closed (thick-walled structures), interconnected (open-cell structures) or both types (thin-walled structures) of porosity. To this end, calculation models of the real materials were directly based on computed tomography (CT) data in order to achieve a high level of geometrical accuracy.

Keywords Cellular metal, thermal conductivity, Maxwell, Lattice Monte Carlo, model structure, computed tomography

1. Introduction

Cellular metals are a type of cellular solid generally characterised by a high porosity, that is, they contain a high fraction of pores or enclosed voids. The known properties of cellular metals such as a high ability for energy absorption, good damping behaviour, sound absorption, excellent heat insulation and a high specific stiffness make these materials useful in, for example, the automotive and aerospace industries. Their good damping, sound and energy absorption

characteristics are useful in packaging or in building construction [1]. In Figure 1, some examples of types of cellular metals are given. Cellular metals can be roughly classified with respect to their porosity into open-cell and closed-cell structures. Open-cell structures (cf. Fig 1a) exhibit interconnected porosity, closed-cell (cf. Figs 1b and 1c) structures contain voids that are completely enclosed by cell-walls. In addition, the expression ‘closed-cell’ has been established in the literature, it will be demonstrated that in the context of thermal properties, it is useful to substitute this classification by the two categories: thin-walled (containing predominantly closed cells) and thick-walled (containing exclusively closed cells) structures.

Fig. 1 Cross sections of three cellular metals: a) Open-cell sponge b) Thin-walled aluminium foam, c) Thin-walled Hollow sphere structure (HSS)

Due to their significant technological potential, cellular metals and their thermal properties have been the subjects of extensive research. Lu and Chen addressed the fire retardant properties of cellular aluminium [2]. They conducted analytical and finite element analyses on the effective thermal conductivity of closed-cell foams (in the compass of this paper they are called thick-walled structures) using two dimensional model structures. The simulations showed a good fire resistance of this material class. Using a Lattice-Boltzmann method Wang and Pan [3] investigated the effective thermal conductivity of randomly generated models of open-cell structures. They found a strong contribution of thermal radiation to the heat transfer for high porosity structures. Their conclusion was based on the application of a correction function [4] to estimate the contribution of thermal radiation which improved the agreement of their numerical findings with experimental data. A recent development is the use of computed tomography (CT) data in numerical analysis to achieve a more accurate geometric representation of these materials. Computed tomography analysis on the thermal properties of cellular aluminium was conducted in [5]. Open-cell and closed-cell structures were investigated using a finite element method and a distinct anisotropy was observed in the case of the open-cell structure. In [6] finite element and Lattice Monte Carlo (LMC) analyses were employed to obtain the thermal conductivity of hollow sphere structures, a relatively new type of cellular metal. Good agreement between the two numerical approaches was found. In addition, isotropic thermal behavior could be observed. In addition to these numerical approaches, several experimental analyses have been performed. Boomsma et al. considered the application of metallic foams inside heat exchangers [7]. They found that for a similar pumping power, metallic foam heat exchangers exhibit thermal resistances that are two to three times lower than those of commercially available heat exchangers. Tian et al. have investigated the use of cellular metals inside heat exchangers [8]. They focused on the effect of cell topology on the fluid flow and heat transfer inside porous copper heat exchangers. Paek et al. [9] conducted measurements on open-cell aluminium foams. They observed that the effective thermal conductivity is widely independent of the foam cell size. Solórzano et al. [10] performed comprehensive experimental measurements on aluminium foams using the transient plane source method. Further measurements were performed by Dukhan and Chen [11] who used a constant heat flux technique for their experimental tests. (Results of these analyses will later be used for comparison with the numerical findings of the present paper.) Zhao et al. [12] considered the temperature dependence of the effective thermal conductivity of open-cell foams in the temperature range between 300 and 500K. They found a rapid increase in thermal conductivity with increasing temperature.

The present paper reports on results of a recently extended numerical method, called the Lattice Monte Carlo (LMC) method, towards the thermal analysis of these advanced materials. In addition, analytical relations are developed and tested to predict the dependence of the thermal properties on the morphology and porosity of cellular structures.

2. Lattice Monte Carlo in thermal analysis

Heat transfer is brought about by three mechanisms: thermal radiation, convection and conduction. The current study aims for the characterization of material behavior at typical ambient temperatures and therefore the effect of radiation is small and may be disregarded [2]. Furthermore, many cellular metals exhibit a low fraction of interconnected porosity and bulk convective heat transfer is not a major component of thermal transport. However, in cellular metals with a high volume fraction of interconnected porosity and high pressure gradients, convective heat transfer is of significant importance and accordingly the present results cannot be applied to such cases. Accordingly, we focus on thermal heat transfer behavior that is governed by thermal conduction alone. Fourier's law relates the heat flux $\dot{Q}/A$ and the temperature gradient $\Delta T/\Delta x$ by multiplication with the effective thermal conductivity λ_{eff} :

$$\frac{\dot{Q}}{A} = \lambda_{\text{eff}} \cdot \frac{\Delta T}{\Delta x}. \quad (1)$$

The effective thermal conductivity λ_{eff} depends on the geometry of the cellular structure and the thermal conductivity λ_w of the cell-wall material. In order to decouple the influence of the cell-wall material, effective thermal conductivities are expressed as a percentage of λ_w . Numerical analyses are conducted using a recently developed Lattice Monte Carlo method [13,14]. In principle, other numerical methods such as the finite element method (yielding shorter calculation times) could be selected instead. However, the LMC method exhibits some significant advantages, in particular a more efficient usage of computer memory and simple model generation that allows the employment of high-resolution models for calculation. As an example, finite element analysis of the computed-tomography models (resolution 800^3 voxels) requires a time-intensive model generation (i.e. testing of numerical convergence and the mesh-independence of the solution) and at least 32 GB of RAM for processing. In contrast, LMC analysis of the same geometries can be conducted on a simple desktop system (2 GB of RAM). The LMC model generation is restricted to a direct translation of the CT voxel data to Lattice nodes.

The basic principle of the LMC method is the directing of lattice-based random walks of small thermal energy parcels that simulate thermal diffusion. The random walks are directed by intersite jump probabilities which are in effect scaled local thermal conductivities. A sufficiently large number of particles (approximately 10^6) are allowed to 'explore' the structure for a certain time t . The effective thermal diffusivity D_{eff} of a structure is then obtained by simply evaluating the average mean square displacement $\langle R^2 \rangle$ of these particles using the Einstein equation in d dimensions:

$$D_{\text{eff}} = \frac{\langle R^2 \rangle}{2 \cdot d \cdot t} \quad (2)$$

which can readily be transformed to the effective thermal conductivity λ_{eff} .

Figure 2 shows a schematic of the LMC algorithm. Prior to the random walk (used for the simulation of energy diffusion), energy parcels are randomly distributed inside the lattice model. As a result, every lattice site exhibits a similar number of initial parcels. Next the random walk loop commences. To this end, an energy parcel is randomly chosen and a jump direction is determined. The three-dimensional lattice models exhibit a primitive cubic topology and accordingly one out of six possible jump directions can be randomly chosen. Based on the conductivities of origin and destination nodes, a local conductivity λ_j for the jump is calculated and converted into a jump probability according to $p_j = \lambda_j / \lambda_{\text{max}}$, where λ_{max} is the maximum conductivity in the model. Subsequently, the jump probability is compared to a uniformly distributed random number $0 \leq \chi < 1$. If the random number is smaller than the jump probability, the particle coordinates are updated before the simulation time t_{LMC} is increment and the next particle is chosen. Further information on thermal LMC analysis can be found [13,14].

Fig. 2 Schematic of the LMC algorithm

In the compass of the numerical LMC analysis, various calculation models are addressed and are introduced in the following. The resolution of the calculation models must be sufficiently large to capture all geometric details. In the case of computed tomography models this is achieved by a direct translation of each voxel to a lattice node. Typical CT calculation models contain in the order of 800^3 nodes. At the same time, the size of the calculation models determines the LMC simulation time. The explanation is that each energy particle must be allowed a sufficient time to explore a representative fraction of the geometry (a typical measure is a half of the model side length). Considering Eq. (2), it can be seen that the required simulation time increases with the square of the side length. Model structures are modeled with a resolution of 200^3 nodes thus requiring only 1/16 of the calculation time of the CT models.

The models are structured according to the categories: open-cell, thick-walled and thin-walled structures. In the literature, thick- and thin-walled structures are normally referred to as closed-cell structures. However, computed-tomography analysis reveals that some of these materials in fact exhibit interconnected porosity (as an example cf. Fig. 5b) and should therefore not be referred to as ‘closed’ structures. Furthermore, it will be shown in the results section below that thin-walled and thick-walled structures exhibit different thermal properties that are uniform within each category. Thin-walled structures exhibiting closed as well as open pores can be distinguished from thick-walled structures exhibiting only closed pores using computed tomography analysis.

2.1 Open-cell Structure

Open-cell structures exhibit predominantly interconnected porosity. Two different simplified model structures are shown in Figs 3a and 3b. In the carcass model, material is concentrated along three orthogonal axes. This is mimicked by the inverted body centred cubic (BCC) structure that is obtained by removing spheres arranged in a BCC pattern from a solid body. Figure 3c shows a computed tomography (CT) reconstruction of the M-Pore[®] foam used for numerical LMC analysis. M-Pore[®] is a commercially available (m-pore GmbH) metallic sponge manufactured by a casting process out of metals such as aluminium or copper.

Fig. 3 Open-cell structures: a) carcass model, b) inverted bcc model, c) M-Pore[®]

2.2 Thick-walled Structure

The thick-walled structures of the numerical LMC analysis are displayed in Fig. 4. Figure 4a shows the cubic inclusion structure which is also used in the analytical approach (10). The material is concentrated along three orthogonal planes and no interconnected porosity exists. The model with spherical inclusions (cf. Fig. 4b) is similar to the inverted BCC model illustrated in Fig 3b. However, the radii of the spheres removed from the solid volume are now chosen to be small enough so that no interconnected porosity is formed. Figure 4c shows a CT reconstruction of a hollow sphere structure (HSS). The matrix is represented in light grey and the metallic spheres in darker grey colors. Within this analysis, the thermal material properties of matrix and metallic spheres are identical ($\lambda_w = \text{const.}$). Hollow spheres are manufactured in a sintering process [15]. Typical base materials are steel and magnesium alloys.

Fig. 4. Thick-walled structures: a) cubic inclusion model, b) spherical inclusion model, c) syntactic HSS

2.3 Thin-walled Structure

Thin-walled structures exhibit both interconnected and closed porosity. In fact, most cellular metals belong to this group since manufacturing processes often introduce small holes or fractures in cell-walls that would otherwise form a closed pore (cf. Fig 5b). Figure 5 shows CT reconstructions of three different materials: Alporas[®], AlSi7 foam and a sintered hollow sphere structure. The chemical composition of the commercial Alporas[®] foam is 97% Al, 1.5% Ca and 1.5% Ti [16].

Fig. 5 Thin-walled structures: a) Alporas[®], b) perforated cell-walls of Alporas (detail), c) AlSi7 foam, d) sintered HSS (detail).

3. Analytical approach

In parallel with the numerical analyses, analytical relations for a reliable prediction of the effective thermal conductivity of cellular metals were tested. The well-known bounds for two phase (i.e. cell-wall material and pores) composite materials are the arithmetic mean (upper bound):

$$\lambda_{\max} = (1 - f_w)\lambda_{\text{Air}} + f_w\lambda_w \quad (3)$$

and the harmonic mean (lower bound):

$$\lambda_{\min} = \frac{1}{\frac{1 - f_w}{\lambda_{\text{Air}}} + \frac{f_w}{\lambda_w}}. \quad (4)$$

The conductivities of the cell-wall material and pore (air) are designated λ_w and λ_{air} , the volume fraction of the cell-wall material is f_w . However, due to the large difference in the thermal conductivities of air and metal (i.e. $\lambda_{\text{air}} = 0.02569 \text{ W/(m K)}$ [17], aluminium $\lambda_w = 167 \text{ W/(m K)}$ [18]) these bounds are much too inaccurate for most cellular metals. For the given values and $f_w = 0.5$ the lower and upper bounds are $\lambda_{\min} = 0.0514 \text{ W/(m K)} < \lambda_{\text{eff}} < \lambda_{\max} = 83.51 \text{ W/(m K)}$. The physical equivalent to these bounds is a parallel (upper bound) or perpendicular (lower bound) configuration of the two phases. LMC analyses of these geometries yield $\lambda_{\min} = 0.0515 \pm 0.0002$ and $\lambda_{\max} = 83.54 \pm 0.27 \text{ W/(m K)}$ which is in good agreement with the analytical solutions. In order to improve the accuracy, we will consider the Series-Parallel analytical approach: first we need to choose the direction of the thermal flux; then we will use a ‘slicing’ technique where we appropriately cut the structure along the direction of the flux and use the analogue of Eqn 4 to calculate the effective conductivity of each slice and then the analogue of Eqn 3 to combine all of the slice’s effective conductivities into the effective conductivity of the total structure. This approach was first used to the open-cell model structure by Dulnev [19]. For the closed-cell model structure this approach was described on numerous occasions; see for example [20].

3.1 Open-cell Structure

For the open-cell structure we will use the geometrical model presented in Fig. 6 where an elementary unit cell is shown. With the characteristic distances d and L (their meaning is clear from Fig. 6) we introduce the ‘linear’ fraction of the metal phase as $\varepsilon_{\text{open}} = d/L$. The volume fraction of the metal phase f_w will be related to $\varepsilon_{\text{open}}$ as:

$$f_w = \varepsilon_{\text{open}}^2 (3 - 2\varepsilon_{\text{open}}) \quad (5)$$

Fig. 6 Open-cell model for the analytical approach.

Then we will have our elementary unit cut into 4 slices along the direction of the heat flux: one ‘solid’ single-phase (metal) bar with the dimensions $d \times d \times L$, one single-phase (air) bar with dimensions: $(L-d) \times (L-d) \times L$ and two identical double-phase plates with dimensions $d \times (L-d) \times L$. We will denote the effective thermal conductivity of the plates as λ_{12} , which is given by:

$$\lambda_{12} = \frac{1}{\frac{1 - \varepsilon_{\text{open}}}{\lambda_{\text{Air}}} + \frac{\varepsilon_{\text{open}}}{\lambda_{\text{w}}}} \quad (6)$$

Then the effective thermal conductivity λ_{open} of the total open structure will be given by:

$$\lambda_{\text{open}} = \varepsilon_{\text{open}}^2 \lambda_{\text{w}} + (1 - \varepsilon_{\text{open}})^2 \lambda_{\text{Air}} + 2\varepsilon_{\text{open}}(1 - \varepsilon_{\text{open}}) \lambda_{12} \quad (7)$$

3.2 Thick-walled structure

For the thick-walled structure (exhibiting only closed porosity) we will use the geometric model presented in Figure 4a. We again introduce L as the width of the elementary unit cell and d as the width of the metal walls of the cell. Then the ‘linear’ fraction of the metal phase can be defined as $\varepsilon_{\text{closed}} = d / L$ with the volume fraction of the metal phase f_{w} related to $\varepsilon_{\text{closed}}$ as:

$$f_{\text{w}} = 1 - (1 - \varepsilon_{\text{closed}})^3 \quad (8)$$

We again cut the elementary unit cell into three slices: one single-phase plate (metal) with dimensions: $d \times L \times L$, similarly a single-phase plate (metal) but with dimensions: $d \times (L-d) \times L$ and a double-phase bar with dimensions: $(L-d) \times (L-d) \times L$. We denote the effective conductivity for the double-phase bar as λ_{21} , which is given by:

$$\lambda_{21} = \frac{1}{\frac{1 - \varepsilon_{\text{closed}}}{\lambda_{\text{Air}}} + \frac{\varepsilon_{\text{closed}}}{\lambda_{\text{w}}}} \quad (9)$$

Then the effective thermal conductivity λ_{closed} of the total structure will be given by:

$$\lambda_{closed} = (2\varepsilon_{closed} - \varepsilon_{closed}^2)\lambda_w + (1 - \varepsilon_{closed})^2\lambda_{21} \quad (10)$$

4. Results

In the following, results of model structures are compared to CT models of real materials and analytical models. The findings are structured according to the categories: open-cell, thick-walled and thin-walled structures.

4.1 Open-cell structure

In Figure 7, the effective thermal conductivities of open-cell structures are plotted versus relative densities. Let us first consider low relative densities $\leq 10\%$. Inside this range, the solutions of the carcass model and the inverse BCC model show only a small deviation. In addition to the model structures, a data point is added for the CT M-Pore[®] model. It is found that the thermal conductivity of M-Pore[®] is best approximated by the carcass model structure. A likely explanation is that both structures can be conceived as being assembled from networks of thin rods. In contrast, the inverted BCC structure exhibits a more uniform material distribution and approximates a thin-walled structure for higher relative densities. At relative densities $> 10\%$, a systematic deviation between the numerical models develops. Experimental values obtained by Dukhan et al. [11] are in reasonable agreement with the numerical carcass model results. In addition to the numerical data, the analytical solution Eq. (7) is added as a dashed line in the same figure. Comparison with the numerical models shows somewhat lower conductivities at higher relative densities. However, the analytical solution shows excellent agreement with the numerical M-Pore[®] CT model (this study) and the experimental data [11]. Accordingly, the analytical approach (7) appears to provide an accurate estimation of the effective thermal conductivity of open-cell structures.

Fig. 7. Effective thermal conductivity of open-cell structures

4.2 Thick-walled structures

The effective thermal conductivities of thick-walled structures are shown in Fig. 8. The curve of the cubic inclusion model is a linear function of the relative density. The spherical inclusion model exhibits similar results but shows slightly lower values for high relative densities. The syntactic hollow sphere CT model is in excellent agreement with the spherical inclusion model. It can be concluded that the stochastic arrangement of pores does not strongly affect the effective thermal conductivity of this type of structure. This confirms the findings of [21] where the effective thermal conductivities of hollow sphere models were calculated for different types of cubic symmetry. In addition, the analytical solution (10) is drawn as a dashed line and excellent agreement with the numerical data is found.

4.3 Thin-walled structures

The effective thermal conductivities of thin-walled structures are plotted in Fig. 9. A distinct dependence on the relative density can be observed. Alporas[®] and the sintered HSS exhibit similar relative densities and almost identical thermal conductivities. In the case of the AlSi7 foam, four different CT data sets with different relative densities were available. The plot shows the thermal conductivity as a linear function of the relative density. Extrapolation of this function yields good agreement with the results obtained for the sintered HSS and Alporas[®]. Comparison with the experimental data obtained by Solórzano et al. [10] shows reasonable agreement. The numerical results seem to form an upper bound for the experimentally obtained conductivities. A possible explanation for this slight deviation is that a different cell-wall conductivity λ_w was assumed. Experimental results from Babcsán et al. [22] are in excellent agreement with the numerical data.

Fig. 8 Effective thermal conductivities of thick-walled structures

Fig. 9 Effective thermal conductivity of thin-walled structures.

5. Discussion

In the following, the results of the previous section are discussed. It should be emphasized here that these findings are only valid as long as the contribution of thermal radiation and convective heat transfer to the thermal transport can be disregarded. However, the good agreement between experimental and numerical data suggests that this assumption is valid for the materials considered. A correction function to account for thermal radiation as suggested in [4] does not seem to be necessary and would in fact deteriorate the agreement.

Figure 10 shows the analytical solutions found for open-cell (7) and thick-walled (10) structures as dashed and full lines, respectively. In addition, data points obtained in the LMC analysis of CT models and experimental measurements [10,11,20] are added. The lowest effective thermal conductivities are found for open-cell structures. At low relative densities, thin-walled structures exhibit thermal conductivities similar to the open-cell ones. Almost identical results are obtained for the CT models of M-Pore[®] (open-cell), Alporas and sintered hollow sphere structures (both thin-walled). The analytical solutions indicate that a systematic deviation between open-cell and thick-walled structures is developed for larger relative densities. The highest effective thermal conductivities at all relative densities are found for thick-walled structures.

Fig. 10 Effective thermal conductivities of cellular structures: analytical, numerical and experimental data.

It can be observed that the two analytical solutions derived for open-cell (7) and thick-walled structures (10) form excellent bounds for the prediction of the effective thermal conductivity of cellular materials. The conductivities of the thin-walled structure lie between these limits and may be estimated based on the linear fit shown as the dotted line in Fig. 10.

Conclusions

This paper focused on the effective thermal conductivity of cellular metals. In this study, the classical distinction between open-cell and closed-cell structures was extended and cellular metals were subdivided into the three categories: open-cell, thin-walled and thick-walled structures. Numerical results were obtained using a Lattice Monte Carlo method and good agreement with the experimental data taken from the literature was observed. The highest thermal conductivities were found for thick-walled structures followed by thin-walled and open-cell foams. Two different types of geometries, namely model structures and computed tomography reconstructions, were addressed within the numerical analysis. It was found that simplified model structures and ‘real’ geometries within the same category (i.e. open-cell, thin-walled or thick-walled) exhibit similar thermal conductivities. In addition to the numerical analysis, an analytical averaging method was used and formulae to describe the effective thermal conductivities of open-cell and thick-walled structure were derived. Excellent agreement with numerical and experimental results was found. The analytical solutions also offer accurate bounds for the upper (thick-walled model) and lower (open-cell model) bounds of the effective thermal conductivity of cellular metals in dependence on their relative density.

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