

## The Mathematical Model of Solid Structural Unit Heat Distribution Based on the Cluster Approach

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The solid structural unit heat distribution mathematical model based on the cluster approach according to the heterogeneity of physical parameters: the thermal conductivity, heat capacity, density and temperature, allowing to obtain the scaling matrix corresponding to these values in the stationary state, enabling calculation of the transient processes in any cluster, allowing to obtain the temporal dependence of these quantities in the corresponding coordinate in the direction of heat propagation for crystalline (with known crystal lattice) and amorphous (with known density) microstructures is presented.

**Keywords:** Cluster model, Thermal conductivity, Heat capacity, Structural unit, Environment heterogeneity

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### 1. INTRODUCTION

The problem of physical properties and processes studying, occurring in solids at nano- and micro-sized levels, exposed to the outside temperature and deformation effects, is quite relevant today, as the development of mathematical models of these processes to be used in predictive calculations and thermal studies of various substances.

In [1-3] the heat propagation mathematical model in a homogeneous structural unit was presented. In that case, density and other physical parameters of the solid were taken to be isotropic-uniformly distributed over the volume of the body, that is, in a given model were in fact independent of space and time variables. As a result of computer simulation based on actual physical parameters (density, the physical dimensions of the structural unit and thermodynamic properties) of the substance temperature distribution in the sample depending on the phase of the thermal process was obtained and the time frame transients in real metals were calculated. However, more accurate calculation of the thermodynamic processes occurring in the simulated and real-world environments requires consideration of the heterogeneity of the substance, as well as the time dependence of the physical parameters. This will allow the in future simulate the real thermal processes in crystalline structures, which will produce more accurate thermophysical calculations.

### 2. MODEL CALCULATION

The purpose of this work is the development the mathematical model of thermal expansion in the structural unit taking into account its heterogeneity and dependence of the physical properties of matter on temperature and time phase of heat process.

In order to be able consider the heterogeneity of the substance, the modeled structural unit is required to split into clusters such that each cluster includes a some atoms belonging to the structural unit (Figure 1).

The cluster size depends on the configuration of the

structural unit: the case for the cubic structure is reasonable to take it equal  $a^3/2$ , for the face-centered and the body-centered structures, respectively  $a^3/3$ . For more complicated configurations the partition will be different depending on the particular mass distribution. This model is also applicable to amorphous solids, taking into account the density uniformity.

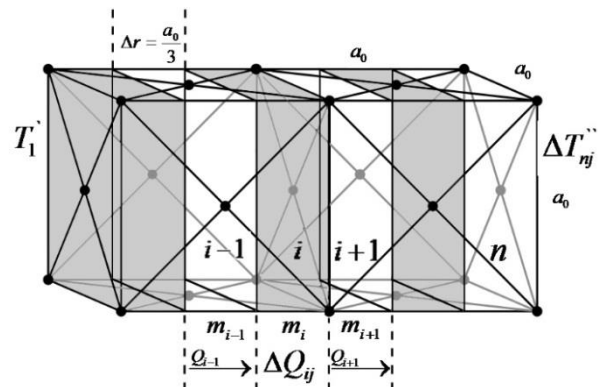


Fig.1 – Structural unit divided by clusters

Proceeding from a principle of the mass additivity, total density of matter in the cluster must match the integral density of the structural unit, which corresponds to the integral density of all the matter. Physical properties of the substance within each cluster, at an initial temperature  $T_0$ , at the initial moment must comply with the following expressions:

$$c_0 = \sum_1^n c_{0i}; \lambda_0 = \sum_1^n \frac{\rho_i}{\rho_0} \lambda_{0i}; \sum_1^n \frac{\rho_i}{\rho_0} = 1 \quad (1)$$

where  $c_{0i}, \lambda_{0i}, \rho_i$  – heat capacity, thermal conductivity coefficient, density in  $i$  cluster at  $T_0$  and  $\tau = 0$ .  $c_0, \lambda_0, \rho_0$  – the integral values of variables.

It will be assumed that on the surface the first cluster temperature is kept constant  $T_1 = T_0 + \Delta T_1$ . Neces-

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sary to find the distribution of temperature in each cluster  $i = 1, 2, 3...n$  at the time  $\tau$ , the amount of heat accumulated therein in a given period of time, the cooling speed and the temperature gradient at the outlet of the corresponding cluster.

The system of equations describing the conservation of enthalpy in clusters in the temperature increments  $\Delta T_{ij}$ , taking into account  $\Delta T_{ij} = \Delta T_{i-1,j}$  (where only bar means the value one at the input, two bares – at the output of the cluster) can be written as:

$$\left\{ \begin{array}{l} \frac{d\Delta T_{1j}}{d\tau} + A_{1j}\Delta T_{1j} = \Delta T_{1j} \\ \frac{d\Delta T_{2j}}{d\tau} + A_{2j}\Delta T_{2j} = \Delta T_{1j} \\ \dots\dots\dots \\ \frac{d\Delta T_{nj}}{d\tau} + A_{nj}\Delta T_{nj} = \Delta T_{(n-1)j} \end{array} \right. \quad (2)$$

for the initial conditions  $\tau = 0, \Delta T_{i0} = 0,$

$$A_{0i} = \frac{\lambda_{0i}}{c_{0i}\rho_i\Delta r^2} = const, \text{ for a given time period } \Delta\tau.$$

In general for any time point  $\tau_j$  solution of (2) takes the form:

$$\Delta T_{ij} = \Delta T_{1j} \left[ 1 + \sum_{i=1}^n \frac{\prod_{j=1}^i A_{ij} e^{P_{ij}\tau_j}}{\|f_i(A_{ij} + P_{ij})\|} \right] \quad (3)$$

where  $|\Delta T_{ij}|$  – matrix of temperature increment changes at the outlet of  $i$  cluster at any point in time,  $|A_{ij}|$  – A constant matrix of changes in  $i$  cluster for the given period of time  $j$ .

$$|\Delta T_{ij}| = \begin{vmatrix} \Delta T_{11} & \Delta T_{12} & \Delta T_{1j} \\ \Delta T_{21} & \Delta T_{22} & \Delta T_{2j} \\ \Delta T_{31} & \Delta T_{32} & \Delta T_{3j} \\ \dots & \dots & \dots \\ \Delta T_{n1} & \Delta T_{n2} & \Delta T_{nj} \end{vmatrix}; |A_{ij}| = \begin{vmatrix} A_{11} & A_{12} & A_{1j} \\ A_{21} & A_{22} & A_{2j} \\ A_{31} & A_{32} & A_{3j} \\ \dots & \dots & \dots \\ A_{n1} & A_{n2} & A_{nj} \end{vmatrix} \quad (4)$$

The diagonal matrix of the whole body parameters:

$$\|f_i(A_{ij} + P_{ij})\|_j = diag |A_{ij} + P_{ij}|_j = \prod_{i=1}^n (A_{ij} + P_{ij})_j \quad (5)$$

$i = 1, 2, 3...n$   
 $j = 1, 2, 3...m$

$P_{ij}$  – eigenvalues of the matrix  $|A_{ij} + P_{ij}|$ ,  $A_{ij} = 0$ , at  $i \neq j$ .

Speed of change outlet temperature increment  $i$  cluster at any moment of time  $j$ :

$$\left| \frac{d\Delta T_{ij}}{d\tau} \right| = \frac{d}{d\tau} |\Delta T_{ij} - \Delta T_{i-1,j}| \quad (6)$$

The temperature gradient in corresponding cluster at any given time can be written as:

$$\frac{d\Delta T_{ij}}{dr} = \left| \frac{\Delta T_{ij} - \Delta T_{i-1,j}}{\Delta r} \right|_j = \frac{d}{dr} |\Delta T_{ij}| - \frac{d}{dr} |\Delta T_{i-1,j}| \quad (7)$$

The amount of heat accumulated in the cluster during the time interval  $(\tau_j - \tau_{j-1})$ :

$$|\Delta Q_{ij}| = |\rho_i \cdot c_{i,j-1}| \cdot \alpha_0^2 \Delta r \left[ \frac{d}{dr} |\Delta T_{ij}| - \frac{d}{dr} |\Delta T_{i-1,j}| \right] \quad (8)$$

However  $|\Delta Q_{ij}|$ :

$$|\Delta Q_{ij}| = |\lambda_{ij}| \alpha_0^2 \left| \frac{d\Delta T_{ij}}{dr} \right| \quad (9)$$

Let us turn to increment of  $c_{ij}, \lambda_{ij}$ :

$$|c_{ij}| = |c_{0i} + c_{ij}|; |\lambda_{ij}| = |\lambda_{0i} + \lambda_{ij}| \quad (10)$$

Interrelation of the specific heat increment in corresponding cluster and the the thermal conductivity coefficient, at any moment of time, using (6), (7), (8), (9), (10) can be represented as:

$$\begin{aligned} |c_{0i} + c_{ij}| \cdot |\rho_i| \Delta r \cdot \frac{d}{dr} |\Delta T_{ij} - \Delta T_{i-1,j}| &= \\ = |\lambda_{0i} + \lambda_{ij}| \cdot \frac{d}{dr} |\Delta T_{ij} - \Delta T_{i-1,j}| \end{aligned} \quad (11)$$

Shall use the notion of thermodynamic heat capacity as the amount of heat supplied to the body  $\Delta Q_{ij}$ , relatedness to the increment of the temperature of the body  $\Delta \bar{T}_{ij}$ .  $\Delta \bar{T}_{ij}$  – shall mean the change of the average integral temperature  $i$  cluster at  $j$  time moment. Accordingly, the increment of the specific heat  $i$  cluster at any time moment  $j$ :

$$\Delta c_{ij} = \frac{\Delta Q_{ij}}{m_i \Delta \bar{T}_{ij}} \Delta \tau \quad (12)$$

where  $\Delta \bar{T}_{ij} = \frac{\int_0^{\Delta\tau} (\Delta T_{ij} - \Delta T_{i-1,j}) d\tau}{\Delta\tau}$ ,  $m_i$  – mass of  $i^{th}$  cluster.

Substituting the expression (12) in (10), we obtain change of the specific heat of the cluster over time:

$$|c_{ij}| = |c_{0i}| + \frac{\Delta\tau}{m_i} \left| \frac{\Delta Q_{ij}}{\Delta \bar{T}_{ij}} \right| \quad (13)$$

Using (13) and (11) obtain the increment of the thermal conductivity coefficient of the cluster at any given time:

$$\begin{aligned} & \left( |\lambda_{0i}| + |\lambda_{ij}| \right) \frac{d}{dr} \left| \Delta T_{ij}^{\infty} - \Delta T_{i-1,j} \right| = \\ & = \left( |c_{0i}| m_i + \left| \frac{\Delta Q_{ij}}{\Delta \bar{T}_{ij}} \right| \right) \frac{d}{d\tau} \left| \Delta T_{ij}^{\infty} - \Delta T_{i-1,j} \right| \end{aligned} \quad (14)$$

Equation (14) determines interrelation of heat capacity and heat conductivity coefficient in corresponding cluster at any given time.

## CONCLUSIONS

The mathematical model of heat distribution in clusters of structural units of the substance, considering heterogeneity of thermal quantities  $c_{ij}, \lambda_{ij}, \rho_i, \Delta T_{ij}$  the direction of propagation thermal energy allows to

investigate interrelation of these variables over time. Using (3-14) in conjunction with (1) makes it possible, using a limit transfer  $\lim_{j \rightarrow \infty} \left| \sum_1^n c_{ij} \right| \in c_0, \lim_{j \rightarrow \infty} \left| \sum_1^n \lambda_{ij} \right| \in \lambda_0$  to

obtain a matrix conformity of these values in the stationary state. Also, the presented model allows to calculate the the transient processes in each of the clusters for thermal quantities  $\Delta c_{ij}, \Delta \lambda_{ij}, \Delta Q_{ij}, \Delta T_{ij}^{\infty}$ . Moreover, the model allows to obtain the dependence of these quantities on time in the given coordinate in the direction of heat propagation and explore these regularities. The model is versatile for crystalline solids, if sufficiently known the inner structure, and amorphous solids with known density.

## Кластерная модель распространения тепла в структурной единице с учетом неоднородности среды

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Представлена математическая модель распространения тепла в структурной единице твердого тела с учетом неоднородности физических параметров: теплопроводности, теплоемкости, плотности и температуры на основе кластерного подхода. Это позволило получить масштабирующую матрицу соответствия этих величин в стационарном состоянии, рассчитать переходные процессы в произвольном кластере, получить зависимость этих величин от времени в соответствующей координате по направлению распространения тепла для кристаллических (с известной решеткой) и аморфных (с известной плотностью) микроструктур.

**Ключевые слова:** Кластерная модель, Теплопроводность, Теплоемкость, Структурная единица, Неоднородная среда.

## Кластерна модель розповсюдження тепла в структурній одиниці з урахуванням неоднорідності середовища

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Представлено математичну модель поширення тепла в структурній одиниці твердого тіла з урахуванням неоднорідності фізичних параметрів: теплопровідності, теплоємності, густини і температури на основі кластерного підходу, що дозволяє отримати масштабуючу матрицю відповідності цих величин в стаціонарному стані, розрахувати перехідні процеси в довільному кластері, отримати залежність цих величин від часу у відповідній координаті у напрямку поширення тепла для кристалічних (з відомою решіткою) і аморфних (з відомою густиною) мікроструктур.

**Ключові слова:** Кластерна модель, Теплопровідність, Теплоємність, Структурна одиниця, Неоднорідне середовище.

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