Results of thermal modeling of Smart Energy Coating with phase-transition material for independent electricity generation

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Abstract. The modeling for Smart Energy Coating is presented. The coating is able to produce electricity on the surface of pipelines and structural elements. Along with electric output, Smart Energy Coating ensures the stable temperature conditions of work for structures, pipelines and regulating elements. The energy production scheme is based on the Peltier principle and the insulating layer with a phase transition. Thermally conductive inclusions of the inside layer with a phase transition material ensure the stable operation of the Peltier element.

1. Introduction

The increase in the scale of production leads to the topicality of limited natural resources and ways of their rational use that are treated as very important questions. In addition, there are regions with sufficient natural resources, but there are difficulties in their using due to remoteness or climatic conditions. Constructions or pipe lines and installations are used in nonstationary temperature conditions. In this case, emitted heat is lost in the atmosphere.

Often sources of renewable energy with good quality are located far from consumers and it is required to make ways to transfer this energy at a distance.

Existing modern systems of the surface generating energy from the sun have a material and can be applied to the surface. But it has several disadvantages. First of all, it works directly when the sun is shining or using diffuse radiation. Second, it has a narrow spectrum of radiation, which the coating is able to absorb, low efficiency and big cost of structure layers. Even in laboratory conditions where there is practically no loss, the efficiency reaches 55%. A limited lifetime and poor efficiency at temperature increase. The use of non-renewable materials is necessary.

Why not to create a device that will produce energy closer to consumers and to supply energy for using at a necessary time? Thus, the energy will be stored during the time when production exceeds consumption. The design does not require too much initial expenses. It takes energy from the environment and produces energy due to the properties of the coating material. This is possible because it has the properties of materials and design features.

So, one can develop a small dimension of construction for storing energy, saving it in the place of production and using it without a fossil fuel and expensive materials. This coating can be used in building construction, the transport sector and even in space industry.
2. Smart Energy Coating

The Smart Energy Coating is developed as means for generating electricity and heat energy. It can work successfully with a different temperature at boundaries of effective areas. Besides, the Smart Energy Coating provides the stable power generation, saves accumulated heat and compensates a temperature difference for a support of work stability conditions in the future. Constructive features contribute to lengthening of the time for an independent power generation. Special nanostructural elements allow absorbing an excess heat and if necessary, to transfer it to elements with a generation of energy. The working principle of the Smart Energy Coating is explained by following theoretical positions.

One of the work principles is to research and develop a material with the effect of thermoelectric conversion, at which the generation of energy takes place depending on the intensification of heat exchange processes and conditions at surface boundaries.

Processes of energy conversion of such phenomena are direct, it works without additional devices has a great advantage, because in some conditions it is the good way for obtaining energy in a small space where there are no moving mechanisms. It makes the system highly reliable.

The temperature regime must be ensured. It promotes the high efficiency of thermoelectric conversion, as well as the power of the Thermoelectric Generator (TEG). The temperatures of hot and cold surfaces and the heat transfer coefficient of the cooling system are required [1].

The thermoelectric Peltier element (Thermoelectric Cooler, TEC) uses the Peltier effect to create a heat flux between the junction of two different types of materials. It is a thermoelectric heat pump. When operated as a generator, one side of the device is heated to a temperature greater than the other side, and as a result, a difference in voltage will build up between the two sides. The value of thermodynamic effectiveness ratio is Carnot Efficiency.

In many modern installations, it is necessary to take into account the following regularity: the heat transfer intensity makes temperature parameters different from that at the beginning, and the thermodynamic efficiency is reduced.

The authors propose excluding the convective component from the construction of SmartEnergy Coating to reduce the influence of the convection coefficient.

Among modern commercial materials, bismuth telluride Bi$_2$Te$_3$ is commonly used in industry (temperature regime of maximum efficiency of 270-500K), PbTe (temperature regime of maximum efficiency of 550-800K), and Si/Ge (temperature regime of maximum efficiency of 1000-1300K). The usefulness of a material in thermoelectric systems is determined by two factors: a device efficiency and a power factor. These are determined by the material's electrical conductivity, a thermal conductivity, Seebeck coefficient and a behavior under changing temperatures.

The modern nanocomposite material consisting of Bi$_2$Te$_3$ nanocrystals with layer coating C$_{60}$ molecules is known. Properties of nanocomposite materials are generated due to discovered properties of fullerene molecules. At different concentrations, the thermo-emf of the composite material increases with a decreasing of a thermal conductivity [2]. As an example used in the laboratory, there is the Smart Energy Coating, a polyimide substrate that can be measured 54 × 20 × 0.1 mm with a thermoelectric material Bi$_2$Te$_3$. The method of specific quantity of heat has been used for experimental measurements of thermal conductivity for the laboratory sample.

The temperature stability in Smart Energy Coating bases on material with the phase-transition layer. It solves the problem of the stable temperature potential by heat transfer in the phase-transition layer. The process of temperature and pressure changes may be control by influence of some external factors. These are control of heat transfer processes and the thickness of materials.

There are phase transitions processes with discontinuous change of parameters. Changing in the density and entropy of material is the first tipe of the phase transition. In this case, the first derivatives of thermodynamic potentials change rapidly with the help of the intensive parameters of the system. And the most important, primary extensive parameters change: specific volume, amount of stored internal energy, concentration of components, etc. In phase transitions of the first kind, the phase does not change in the whole volume immediately, but gradually with separation (or intake) of a certain
amount of energy. One of foundation principles of alignment for temperature fluctuations and maintaining a stable temperature is based on the solution of Stefan's problem. Thus the location of the main functional elements of the researched layer and their size are determined. A layer with various functional inclusions is located on the boundary of the heat exchange zone and compensates the heat input. At this moment, the physical and textural properties of synthesized suspensions are in the research stage. Let us data of the specific resulted thermal diffusion of materials. It is possible to determine the total amount of functional material amount of latent heat, besides one can test the thickness and form of elements. The mathematical modeling of the Smart Energy coating process was done.

3. The mathematical modeling of nonlinear heat transfer processes for the researched layer

Mathematical models of processes of heat and mass transfer in substance with phase transitions are nonlinear systems of differential equations. An analytic solution of the one-dimensional nonlinear heat conduction problem is called the Stefan problem. A model with constant coefficients of an heat equation due to Stefan type of boundary conditions of phase transition is nonlinear, and the main method of solving is the numerical method. Only in some particular cases it is possible to apply the analytical method. In this case so-called self-similar solutions can be obtained. It is characterized by similarity of spatial parameters of sought-for quantities for non-stationary modes. Such solutions are for one-dimensional problems in the half-space with constant borders and initial conditions. Self-similar solutions allow one to describe experimental processes for long-term characteristics and distances from the boundary. It affects to terminal conditions, but time conditions and distances are far from the critical system stage [5,7].

Let us suppose that a liquid medium is spreading in a half-space $x > 0$. At $t < 0$, the temperature of all layers of the liquid is the same and $u > u^*$, where $u^*$ - a liquid solidification temperature. Commonly it is $u^* = 0$.

From time $t = 0$ at border $x = 0$, a constant temperature is $u_c < 0$ below crystallization temperature $u^*$. In this case, at $t > 0$, a layer of solid phase shows up near a boundary surface, a thickness increases over time (Figure 1). The crystallization front $x = \xi(t)$ separates the solid phase from the liquid phase, moving at some speed $v = d\xi/dt$ to the direction of the liquid phase. It is the problem statement and $\xi(0) = 0$.

![Figure 1. The direction of the crystallization front.](image)

The heat of the phase transfer is emitted after crystallization of the liquid and takes away the energy due to the thermal conductivity of the solid phase through boundary surface $x = 0$.

Let us designate the moving crystallization front by the index "1", these are options of the solid phase, and index "2" - the liquid phase. Then, assuming that properties of the medium change unevenly in the phase transition, one can write the heat equation for two phases:

\[ \frac{\partial T}{\partial t} = \alpha \nabla^2 T \]

Where $\alpha$ is the thermal diffusivity.
\[
\begin{align*}
\frac{\partial u_1}{\partial t} &= \alpha_1^2 \frac{\partial^2 u_1}{\partial x^2}, \quad t > 0, \ 0 < x < \xi(t); \\
\frac{\partial u_2}{\partial t} &= \alpha_2^2 \frac{\partial^2 u_2}{\partial x^2}, \quad t > 0, \ \xi(t) < x < \infty; 
\end{align*}
\]

where \(\alpha_1\) and \(\alpha_2\) - the thermal diffusivity of solid and liquid phases, respectively.

Taking into account the initial moment of liquid phase time has the initial condition for the problem, it is written in the form:

\[u_2(x,0) = \text{const}, \quad x > 0.\]  \hspace{1cm} (2)

Boundary conditions of the problem is:

a) at the boundaries of the region

\[u_1 = u_c = \text{const} < 0 \text{ at } x = 0; \]

\[u_2 \rightarrow u_0 = \text{const} > 0 \text{ at } x \rightarrow \infty;\]  \hspace{1cm} (3)

b) in the front of phase transition

\[k_1 \frac{\partial u_1}{\partial x} \bigg|_{x = \xi^+} - k_2 \frac{\partial u_2}{\partial x} \bigg|_{x = \xi^+} = \rho_1 q^* \frac{df}{dt};\]  \hspace{1cm} (4)

where \(q^*\) - the latent heat of crystallization, concerning the unit mass of the solid phase.

Using self-similar variable \(\eta = \frac{x}{\sqrt{t}}\) (Boltzmann transform), let us transform equations (1) to ordinary differential equations for functions \(u_1(\eta)\) and \(u_2(\eta)\).

Integrating twice and returning to variables \(x\) and \(t\), let us present solutions of equations (1), and after transformation it has the view:

\[\xi(t) / \sqrt{t} = \alpha = \text{const}.\]  \hspace{1cm} (5)

Thus, accurate within certain constant \(\alpha\) representing the coefficient of thermal diffusivity, the law of motion for the phase transition front has the view:

\[\xi(t) = \alpha \sqrt{t},\]  \hspace{1cm} (6)

and its speed

\[v = \frac{d\xi}{dt} = \alpha/2 \sqrt{t}.\]  \hspace{1cm} (7)

It decreases in time, and the layer of the solid phase increases and thickens.

Thus, a nonlinear heat conduction problem with a phase transition can be solved. The task solution uses for the modeling of a heat accumulation and consumption in non-stationary heat exchange process. It concerns the wall and structures of Smart Houses. It may be applied for researches in technological processes of a melting, directed crystallizations, a growing of single crystals and a production of specified structures of semiconductor materials. Using mathematical models these processes can be optimized for various factors.

After solving the Stefan problem for several general cases of boundary conditions and the determining of process characteristics (the reaction rate and the size of material), it is possible to make the mathematical three-dimensional modeling of differential equations for research models, based on the method of finite differences. The modeling of three-dimensional differential equations by the method of finite differences can give a real picture of processes to select the location of working particles to a compensation of temperature fields [7-10].

Stages of modeling include the determination of zones for an inhomogeneous temperature field and the superimposition of a phase-transition material layer [4] to equalize the thermal-field gradient.

The modeling of the phase-transition layer with heat-conducting inclusions is made to exclude the convection transfer and for additional layers of thermal insulation.

As a working medium for providing a thermal regime, a composite heat-accumulating material with paraffin P-2: B-TAM-50 ТУ 1-595-53-592 is taked.

As a polymer base ethylene-propylene rubber with a vulcanizing group is used. The role of the melting substance is the paraffin.

Thermophysical properties B-TAM-50:

- the latent heat of the phase transition, \(r = 117\ \text{KJ} / \text{kg}\);  
- the phase transition temperature, \(T_c = 53\ \text{C}\);
- the density, \( \rho = 900 \text{ kg/m}^3 \);
- the specific heat and thermal conductivity as a function of temperature are presented in Table 1.

**Table 1.** Specific heat and thermal conductivity of the material as a function of temperature T, C

| Temperature | -60 | 0  | 25  | 50  |
|-------------|-----|----|-----|-----|
| \( \lambda \), W/m·K | 0,26 | 0,27 | 0,28 | 0,29 |
| \( C_p \), KJ/kg | 0,5  | 1,4 | 1,7 | 2,1 |

The thermal inclusions is carbon (graphite layers with fibers). In Figure 2 a temperature field is shown near heat-conducting graphite inclusions.

![Figure 2. The modeling of internal layers of the phase-transition layer with heat-conducting inclusions.](image)

The analysis of thermal phenomena with ANSYS programm is made. In the solution of thermal problems, temperature distributions (temperature fields) and heat transferlines (for special cases) in the researched system and its parts were calculated. There are typical thermal quantities for calculations of thermal temperature fields, an amount of heat released or absorption, temperature gradients along the distribution lines of heat-conducting inclusions, and the density of heat fluxes.

The thermal conductive inclusions transfer the necessary amount of a heat flow from the outer layers to inner layers, which are attached to the TEC directly. During a phase change, energy may be added or subtracted from a system, but the temperature will not change. The temperature will change only when the phase change is completed.

Based on the simulation results of this sample, the thickness of thermal inclusions equal to 2 mm was selected for a heat flow equalization. The thermal insulation layer with the phase-transition material inclusions protects from big temperature changes reliably, undesirable heating and cooling of the structure. Inclusions with the phase-transition material ensure the reliable work of the thermocouple.
Figure 3. The modeling of the phase-transition layer with thermal conductive inclusions for apply in the TEC

Figure 4. The phase-transition layer with thermal conductive inclusions.

Figure 4 presents heat-conducting inclusions in constuctions of complex forms. In this simulation, a spherical shape is embedded. It has the similar circular form for the most uniform distribution of thermal lines in graphite conductors with obtained density. In addition, an alternation of the phase-transition layer and the conducting layer allows one to use the functional completely.

Thus, the phase-transition layer with heat-conducting inclusions makes it possible to distribute the temperature field through heat-conducting inclusions. Thus the required value of the temperature difference arises to places with Peltier elements directly. The remaining areas are protected from excessive heat flux reliably.

Figure 5. The schematic representation of thermal inclusions.

In Figure 5 the blue color is the flow of cold coolants, the gray is the heat-insulating material, the black is the thermoelectric element of the Peltier (Thermoelectric Cooler, TEC).

The coating can be used in structures of Siberian and northern zones. There is a temperature difference in systems of heating and the ambient medium. For example, in heat supply systems with a temperature difference of 40-100 degrees, and a temperature drop of 1-3 degrees, there are 3 amperes at a voltage of about 18 volts. The level can be increased using modern film technologies.

4. Conclusion
According to results of thermal modeling and several full-scale experiments, there is a conclusion about the developed heat-insulating layer. It includes a phase-transition material with heat-conducting inclusions and makes it possible to distribute the temperature of the heat field through heat-conducting
inclusions. The level of a temperature difference transfers directly to places with the Peltier elements. Remaining areas are protected from an excessive heat flux reliably. The Smart Energy Coating can be used in structures, in pipelines, solar heating and cooling systems and technical equipment. Also they can be applied in places with temperature losses, in thermal power generation systems. In this case, the output voltage is sufficient for the operation of equipment, lighting, and technique.

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