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COMPUTER DESIGN OF THERMOELECTRIC FGM MATERIALS AND DEVICES ON THEIR BASIS

- **FGM** is the way to increase thermoelectric energy conversion efficiency.
- **FGM** is the prospect for progress achievements when designing the latest thermoelectric products.
- **FGM** are made by irregular impurity distribution along legs and the use of inhomogeneous magnetic fields.
- **FGM** design is a complicated physical and mathematical problem. Institute of Thermoelectricity has elaborated methods of FGM design.
- Computer programs for FGM design are proposed. Programs were elaborated on the base of the mathematical theory of optical control. Programs employ the latest achievements over current carriers and phonons spectra, impurities effect on thermoelectric materials properties. Optimal impurity distributions and distributions of magnetic field strength along the legs are determined from the programs.
- The use of computer design in creation of FGM increases the efficiency of thermoelectric generators based on *BiTe* by 15-25%, *PbTe*, *GeTe* by 15-20%.
- The use of computer design in creation of FGM allows to increase the coefficient of performance of single-stage thermoelectric cooling modules by 20-40%, multi-stage modules - by 1,5-5 times.
- The programs are the basis for creation of thermoelectric FGM technologies.

1.Computer-aided design program of FGM based on *Bi-Te* for thermoelectric cooling under the conditions of maximum temperature drop.

Working temperature range is -150 - +250°C, leg length is within 0.5 - 5 mm. The design results in the optimal inhomogeneity of doping impurities and component percentage in *BiTe-BiSe, BiTe-SbTe* compositions along the legs. The use of computer-aided design for creating FGM leads to the increase in T_{max} at 300 K from 70 K to 90 K and is equivalent to $Z=4.5{\cdot}10^{-3}$ K^{-1}.

2.Computer-aided design program of FGM based on *Bi-Te* for thermoelectric cooling under the conditions of maximum coefficient of performance.

Working temperature range is -150 - +250°C, leg length is within 0.5 - 5 mm. The design results in the optimal inhomogeneity of doping impurities and component percentage in *BiTe-BiSe, BiTe-SbTe* compositions along the legs. The use of computer-aided design for creating FGM leads to 1.5 - 2 fold and greater increase in the coefficient of performance at T_{max} more than 70 K at cooling from 300 K, which is equivalent to $Z = 4.5{\cdot}10^{-3}$ K^{-1}.

3.Computer-aided design program of FGM based on *Bi-Sb* for thermoelectric cooling.

Working temperature range is -200 - -100°C, leg length is within 0.5 - 5 mm. The design results in the optimal inhomogeneity of doping impurities and component percentage in *Bi-Sb* composition along the legs, as well in the optimal inhomogeneity caused by the inhomogeneous magnetic fold perpendicular to the legs within 0 - 5000 Oersted. The program includes two cooling conditions - condition of maximum temperature drop and condition of maximum economy according to the coefficient of performance value. The use of computer-aided design for creating low-temperature FGM leads to the increase in the coefficient of performance by 20 - 40 %, which is equivalent to 2 - 3 fold decrease in electric power of a multi-stage cooler.

4. Computer-aided design program of cascade thermoelectric cooling modules based on FGM.

The program allows to design cascade modules with an arbitrary number of cascades for temperature range of -200 - +250 °C at cooling values 0 - 450 K. Leg length is within 0.2 - 5 mm. The program takes into account commutation and contact electric and heat losses, as well as all kinds of heat transfer to the environments. The program allows to design coolers both from the homogeneous materials and FGM. The program provides; determination of the optimal number of cascades for the assigned temperature range; determination of the optimal intercascade match according to the values of electric and thermal power; determination of the optimal currents and voltages and, accordingly, optimal dimensions of legs and their number in cascades; determination of the optimal compositions of doping impurities and component percentage for multi-component alloys *BiTe-BiSe, BiTe-SbTe* and *BiSb* in each cascade; determination of inhomogeneity function for FGM in each cascade; determination of the optimal number of cascades in combined batteries from thermoelectric cascades and cascades with magnetic field; determination of inhomogeneity functions of magnetic field in low-temperature cascades based on *Bi-Sb* alloys; determination of the optimal FGM on the basis of combined effect of magnetic field and optimal doping. The use of the programs allows to improve the efficiency of multi - cascade cooling modules 1.5 - 5 times, especially for the case of cooling below -100°C.

5. Computer-aided design program of FGM based on *Bi-Te* for thermoelectric generators.

The program provides design for working temperature range 20 - 350°C at leg length within 0.5 - 5 mm. The program determines the optimal function of doping impurity concentration and optimal modifications in *BiTe-BiSe, BiTe-SbTe* alloy compositions for arbitrary working temperature ranges with the purpose of reaching the maximum efficiency or the maximum power. The use of computer-aided design for creating FGM allows to increase the efficiency by 15 - 25 %.

6. Computer-aided design program of FGM based on *Pb-Te, Ge-Te* for thermoelectric generators.

The program provides design for working temperature range 200 - 750°C at leg length within 0.5 - 5 mm. The program determines the optimal function of doping impurity concentration and optimal modifications in *PbTe-GeTe* alloy compositions for arbitrary working temperature ranges with the purpose of reaching the maximum efficiency or the maximum power. The use of computer-aided design for creating FGM allows to increase the efficiency by 15 - 20 %.

7. Computer-aided design program of cascade thermopiles with FGM.

The program provides design of multi-cascade modules with an arbitrary number of cascades from the alloys of *BiTe-BiSe, BiTe-SbTe, GeTe, GeSi* in the temperature range 20 - 1300°C at leg length within 0.5 - 10 mm. The programs take into account commutation electric and heat losses, as well as intercascade heat losses. The program determines: the optimal number of cascades for assigned working temperatures and materials for each cascade; the optimal working temperature ranges for each cascade; the optimal functions of doping impurity concentrations and optimal modifications of substance composition along the legs; the optimal relationships of intercascade electric and heat powers; the optimal number of legs in each cascade, their optimal length and section; the optimal values of efficiency power. The use of computer-aided design for creating cascade generators based on FGM allows to attain record-breaking values of efficiency.

8. Monograph on the optimal control of thermoelectric material properties for creating FGM:

L.I. Anatychuk, V.A. Semenyuk "Optimal Control of Thermoelectric Material and Device Properties", 200 p. The monograph dwells on the theory of thermoelectric phenomena on the inhomogeneous materials, mathematical method -of Pontryagin, optimal control for finding optimal inhomogeneity functions. Classification of all types of problems of optimal control of thermoelectric material inhomogeneity to reach the maximum efficiency, the maximum cooling, the maximum coefficient of performance, the maximum speed. Mathematical methods of program construction for designing the optimal inhomogeneous FGM structures. Examples of FGM computer-aided design. The readers of the monograph can obtain scientific fundamentals of the theory of the inhomogeneous thermoelectric materials and computer-aided design of FGM.

Concerning placement of orders for FGM design, acquisition of computer programs and technologies, development and delivery of the necessary thermoelectric materials and thermoelectric cooling batteries and generators apply to the address at the top of the first page.

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