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A Novel 3D TCAD Simulation of a Thermoelectric Couple configured for Thermoelectric Power Generation

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Abstract. This paper documents the novel design, modelling and 3D simulation of a single thermoelectric couple using the Technology Computer Aided Design (TCAD) semiconductor simulation software package by Synopsys. Preliminary simulation results are presented for thermoelectric power generation, and successfully demonstrate the basic thermoelectric effects, and how the application of a temperature gradient to a thermoelectric couple results in a small amount of electrical power being generated at a load resistor. The TCAD simulation model will enable further investigation in the future into different material structures, thermoelectric couple and module design, and the improvement in efficiency and thermoelectric module performance.

Key words

Thermoelectric, Seebeck, micro-power generation, TCAD, 3D simulation

1. Introduction

This paper begins with a short background review of thermoelectric technology, followed by an overview of a typical thermoelectric module construction, highlighting the main elements and material structure, and a detailed description of a single thermoelectric couple connected for thermoelectric power generation. The 3D modelling of a thermoelectric couple is presented, including preliminary simulation results obtained for the thermal and electrical characteristics of the device when it is connected as a thermoelectric generator. The simulation results are discussed with reference to basic thermoelectric theory, and the paper draws conclusions on the validity and effectiveness of the 3D TCAD thermoelectric couple simulation model.

2. Background

Thermoelectric technology is the focus of significant research and can make an increasing contribution to the need to find alternative methods of power generation, heating and cooling. The technology can also be used in applications where other renewable technologies could not be used, or in combination with other renewable technologies, in order to enhance a systems overall performance. The concept of using thermoelectric technology to generate electrical power from waste heat in a system has been considered for some time, although the technology is often overlooked in discussions surrounding renewable energy sources. This is partly due to the relatively low levels of electrical power generated from a typical thermoelectric module, usually in the milli-watt (mW) or micro watt (µW) range, and a typical conversion efficiency of 5% to 10% [1]. However, with the addition of relatively simple electronic signal-conditioning techniques, for example low-power DC to DC conversion, coupled with electrical storage in supercapacitors, enables the electrical power output from a thermoelectric power generation system to be increased to a useful level, and can output sufficient electrical power to operate low-power electronic systems, recharge or replace batteries in many applications, and is considered an environmentally friendly and renewable energy source. The technology is not limited to low-power applications, with significant focus and research into thermoelectric power generation from waste heat in the automotive market, and is extensively used to provide power to space-craft.

Thermoelectricity utilises the Seebeck, Peltier and Thomson effects that were first observed between 1821 and 1851. Practical thermoelectric devices emerged in the 1960's and have developed significantly since then with a number of manufacturers now marketing thermoelectric modules for power generation, heating and cooling applications [2]. Ongoing research and advances in thermoelectric materials and manufacturing techniques, enables the technology to make a greater contribution to address the growing requirement for low-power energy sources typically used in energy harvesting and scavenging systems.

Commercial thermoelectric modules can be used to generate a small amount of electrical power, typically in the mW or µW range, if a temperature difference is maintained between two terminals of a thermoelectric module [3]. Alternatively, a thermoelectric module can operate as a heat pump, providing heating or cooling of

an object connected to one side of a thermoelectric module if a DC current is applied to the module's input terminals [3].

3. Typical thermoelectric module construction and material structure

A standard thermoelectric module is constructed from several P-type and N-type thermoelectric couples. A single thermoelectric couple is constructed from two 'pellets' of semiconductor material usually made from Bismuth Telluride (Bi_2Te_3). One of these pellets is doped with acceptor impurity to create a P-type pellet, the other is doped with donor impurity to produce an N-type pellet. The two pellets are physically linked together on one side, usually with a small strip of copper, as shown in Fig. 1, and placed between two ceramic plates.

For thermoelectric power generation, if a temperature difference is maintained between two sides of the thermoelectric couple, thermal energy will move through the electrically conductive N-type and P-type pellets. Charge carriers will move through the device with this heat and an electrical voltage, called the Seebeck voltage, will be created. If a resistive load is connected across the module's output terminals, electrical current will flow in the load and a voltage will be generated at the load [4] – [5]. A single thermoelectric couple, connected for thermoelectric power generation, is shown in Fig. 2. Practical thermoelectric modules are constructed with several of these thermoelectric couples connected electrically in series and thermally in parallel. Standard thermoelectric modules typically contain a minimum of three couples, rising to one hundred and twenty seven couples for a larger device [3].

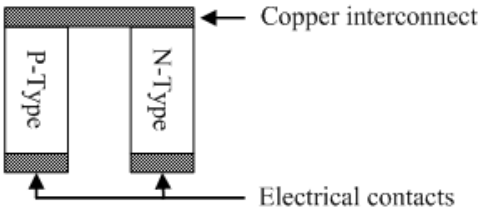

Fig. 1. A standard thermoelectric couple [3]

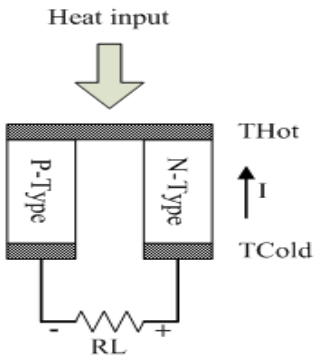

Fig. 2. A single thermoelectric couple connected for thermoelectric power generation [3]

4. Technology Computer Aided Design (TCAD)

The Synopsys TCAD semiconductor simulation package has been chosen for this work as it is widely used in the semiconductor industry to simulate semiconductor device behaviour, and has the capability to simulate semiconductor process and device simulation. The successful modelling of a single thermoelectric couple will provide a platform for further investigation into process simulation, thermoelectric module construction, material structure and performance characteristics. Existing published work into thermoelectric modelling and simulation have emphasised the use of ANSYS and SPICE compatible simulation software. It is anticipated that modelling a thermoelectric couple in TCAD will allow a more detailed analysis of the thermoelectric electrical and thermal effects to be undertaken than has been published in previous studies.

TCAD comprises of a suite of programs that can be executed independently or together in the form of a Workbench project, in order to simulate the electrical characteristics and thermal properties of a device. A simulation project has been created in Sentaurus Workbench in order to control the flow of the simulation, define experiment parameters and variables. Specific TCAD tools have been added to this workbench project in order to create a working simulation. Sentaurus Structure Editor is executed first, and the 3D thermoelectric couple structure is created within this environment, and then meshed using Sentaurus Mesh. This meshed device is then passed to Sentaurus Device, where the electrical and thermal simulation of the device model is executed. The behaviour of the device is simulated numerically by calculating terminal currents, voltage and charges using a set of physical device equations that describe the carrier distribution and conduction mechanisms [6]. The output of Sentaurus Device is then plotted and displayed using Tecplot and Inspect.

5. 3D simulation model of a single thermoelectric couple using Sentaurus Structure Editor

A single thermoelectric couple has been modelled in Sentaurus Structure Editor, and is shown in Fig. 3.

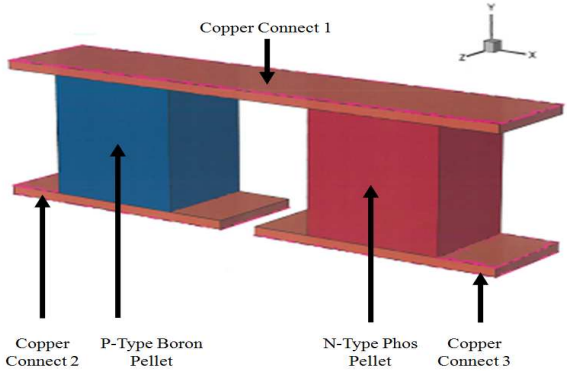

Fig. 3. A 3D single thermoelectric couple modelled in Sentaurus Structure Editor

The P-type material has been simulated using Silicon as the base material, heavily doped with Boron with a constant doping profile and initial concentration of $1e^{+}15cm^{-3}$. This level of doping was chosen in order to create a heavily doped P-type region in the Silicon pellet. The N-type pellet is similarly constructed, using Silicon as the base material, heavily doped with Phosphorus at $1e^{+}15cm^{-3}$. The three copper interconnects are labelled 'Copper Connect 1'; 'Copper Connect 2' and 'Copper Connect 3' respectively.

An electrode contact was made on the face of Copper 2 and Copper 3 to simulate the negative and positive electrical connections to the couple. A thermal contact was made on the face of Copper 1; Copper 2; and Copper 3; in order to allow the temperature of each contact to be specified or calculated, and are shown in Fig. 4. This figure also highlights the dimensions of the thermoelectric couple, and is constructed from the 3D model with a cut-through the device in the Z-direction. The dimension of the 3D device in the Z-direction is 1100 micron metres.

Although most commercial thermoelectric modules use Bismuth Telluride as the base material, as this exhibits the most pronounced thermoelectric effects at room temperature, this paper documents the use of Silicon as the base material for simulation. Silicon has been chosen as the base material as TCAD's physical device equations that describe the carrier distribution and conduction mechanisms, materials database and parameter list is comprehensive for Silicon. Other material structures can be simulated, but it may be necessary to specify specific material parameters that are not listed in TCAD's materials database. If a material is not specified, and it is necessary for TCAD to complete the simulation, TCAD will default to using Silicon parameters which may cause unforeseen device behaviour and results. Once the basic thermoelectric properties have been successfully demonstrated using Silicon, even though this may be at a reduced level than could be seen with state-of-the-art materials, it will be possible to alter the material structure and move to Bismuth Telluride and other material structures with increased confidence.

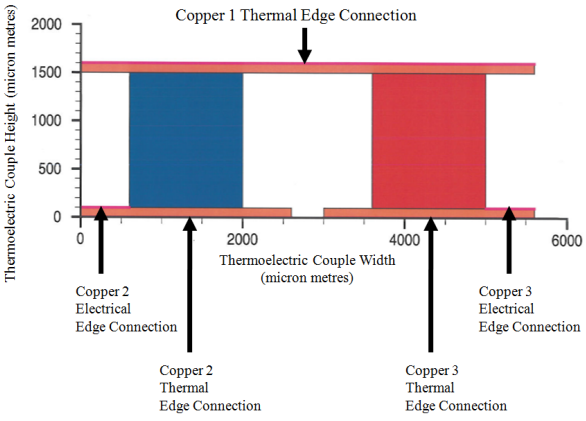

Fig. 4. A cut-through in the Z-direction of the 3D model highlighting the electrical and thermal connections

For thermoelectric power generation, the 3D thermoelectric couple shown in Fig. 3 was simulated as a TCAD 'Mixed Mode Simulation' rather than a 'Single Device Simulation'. In Mixed Mode simulation, it is possible to add external components and circuitry to the 3D device structure designed in Sentaurus Structure Editor, and in this case a load resistor (RL) was connected between the output terminals 'Copper 2' and 'Copper 3' of the device, as shown in Fig. 5, in order to calculate the electrical power generated at the load.

A single thermoelectric couple with ceramic outer plates has also been simulated, and is shown in Fig. 6 and Fig. 7. The top and bottom face of the two ceramic plates have been used as the thermal contacts of the device, and are labelled 'Ceramic top' and 'Ceramic bottom' respectively. Otherwise, the construction of the device is the same as shown earlier for a single thermoelectric couple.

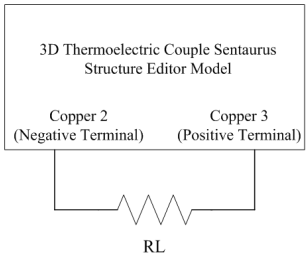

Fig. 5. A schematic representation of the Mixed Mode simulation of a single thermoelectric couple with the load resistance RL connected between the thermoelectric model output terminals

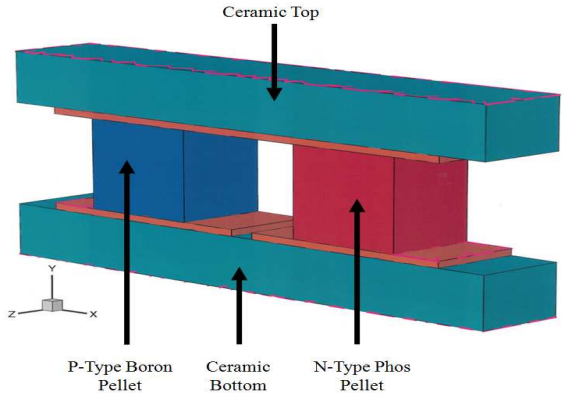

Fig. 6. A 3D single thermoelectric couple with two ceramic outer plates modelled in Sentaurus Structure Editor

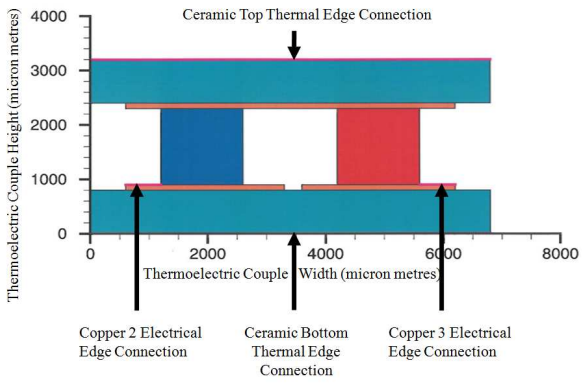

Fig. 7. A cut-through in the Z-direction of the 3D model with ceramic plates, highlighting the electrical and thermal connections

6. Simulation Methodology

The single thermoelectric couple has been modelled in Sentaurus Structure Editor, connected to a load Resistor RL, and tested using a Mixed Mode simulation for thermoelectric power generation. The temperature of the thermal contact on Copper 1 was increased from steady-state conditions of 300 Kelvin to 301 Kelvin. The temperature of the other two thermal contacts, Copper 2 and Copper 3, were kept at 300 Kelvin. This creates a 1 Kelvin temperature difference between both sides of the couple. The load resistance RL was also increased from 10 ohms through to 350 ohms, in 10 ohm steps, in order to establish where maximum power transfer occurs. Maximum power transfer should occur when the load resistance RL is at the same resistance value as the internal resistance of the thermoelectric couple under test. The voltage across the load resistor and the load current was recorded using the simulation program, and the electrical power generated at the load calculated using:

$$P = V \times I \quad \text{measured in Watts} \qquad (1)$$

Where V is the electrical voltage measured across the load resistor RL; and I is the electrical current flowing through the load resistor RL.

The P-type and N-type doping concentration was altered from $1e^{+}15cm^{-3}$ to $1e^{+}14cm^{-3}$ and $1e^{+}16cm^{-3}$ in order to establish if the doping concentration has any effect on the electrical power generated by the thermoelectric couple.

The temperature of the thermal contact on Copper 1 was then increased from 301 Kelvin to 325 Kelvin; 375 Kelvin; and 400 Kelvin. The temperature of the other two thermal contacts, Copper 2 and Copper 3, were kept at 300 Kelvin. This creates a temperature difference between both sides of the couple of 25 Kelvin; 50 Kelvin; 75 Kelvin; and 100 Kelvin respectively.

The simulation tests were then repeated using the model of the thermoelectric couple with ceramic plates, shown earlier in Fig. 6, in order to compare the electrical and thermal characteristics of the two device structures.

7. Simulation Results

For thermoelectric power generation, preliminary simulation results successfully demonstrate that if the thermoelectric couple is subjected to a temperature gradient from one side of the device to the other, an electrical power is generated at the load resistor RL connected between the device output terminals. This is in agreement with the fundamental thermoelectric theory discussed earlier.

With an initial dopant concentration of $1e^{+}15cm^{-3}$ for both P-type and N-type pellets, the temperature of the thermal connection at Copper 1 was increased from 300 Kelvin to 301 Kelvin, with the temperature of the thermal contacts at Copper 2 and Copper 3 maintained at 300 Kelvin. The temperature of the thermoelectric couple's lattice is shown in Fig. 8 under these test conditions, and highlights that a temperature gradient exists within the device.

The electrical power generated at the load is shown in Fig. 9, and is compared with the power generated when no temperature gradient exists and the whole device is at a uniform temperature. It can be seen that without a temperature gradient, there is only negligible electrical power generated at the load, although it is not absolutely zero watts. This is not unexpected as there will be a small amount of natural movement of charge carriers at a room temperature of 300 Kelvin. As the temperature gradient of 1 Kelvin is applied to the device, the output power at the load can be seen to increase to a peak of 0.00563 micro watts with a load resistance of 170 ohms, where maximum power transfer is achieved.

Further tests have been conducted with a modified P-type and N-type doping concentration of $1e^{+}14cm^{-3}$; $1e^{+}15cm^{-3}$; and $1e^{+}16cm^{-3}$; with the results shown in Fig. 10. The temperature at the thermal contacts of Copper 1 was set to 301 Kelvin, and the thermal contacts at Copper 2 and Copper 3 maintained at 300 Kelvin as before.

Changing the doping concentration significantly alters the amount of electrical power generated at the load, and the resistance of the load where maximum power transfer occurs. Increasing the P-type and N-type doping concentration to $1e^{+}16cm^{-3}$ increased the electrical power output of the thermoelectric couple, and decreased the resistance where maximum power transfer occurs. Conversely, decreasing the doping concentration has reduced the amount of electrical power generated at the load resistance and increased the value of load resistance where maximum power transfer is achieved.

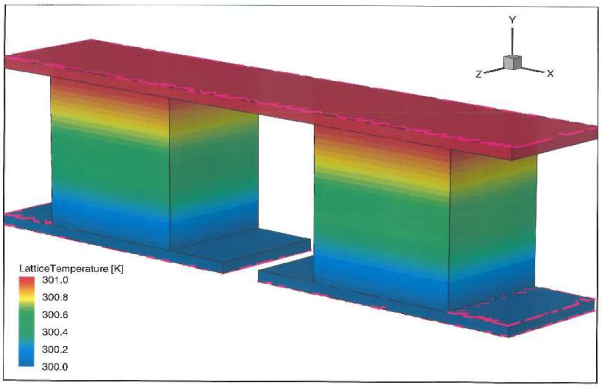

Fig. 8. The lattice temperature for a single thermoelectric couple with an applied 1 Kelvin temperature gradient between both sides of the device

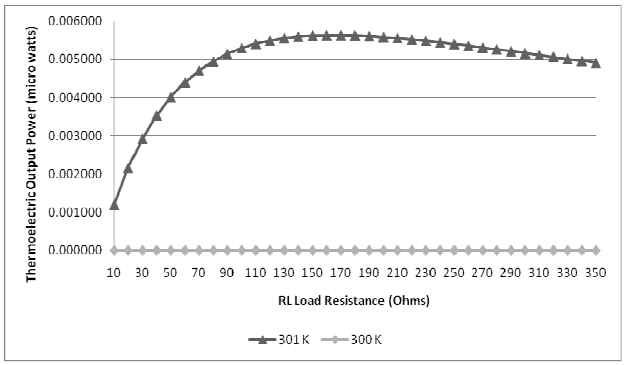

Fig. 9. The electrical power generated at the load resistor (RL) with a temperature gradient of 1 Kelvin between both sides of the device

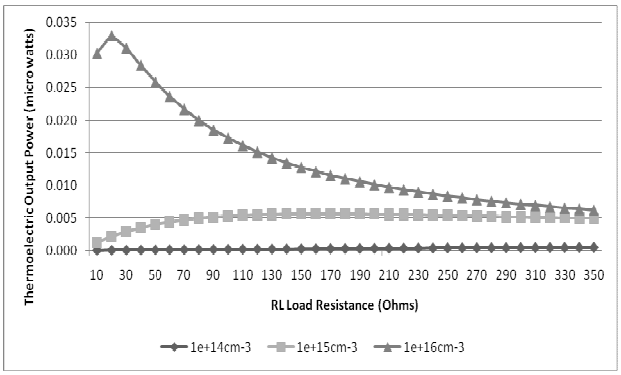

Fig. 10. The electrical power generated at the load resistor (RL) with different P-type and N-type doping concentrations and a 1 Kelvin temperature gradient between both sides of the device

Increasing the thermal gradient on both sides of the device, by increasing the temperature of the thermal contact at Copper 1, results in an increase in electrical power generated at the load, as shown in Fig. 11. This is as expected as the Seebeck effect is temperature dependent [2]. A doping concentration of $1e^{+}16cm^{-3}$ for both P-type and N-type pellets was used for these tests, as earlier results confirmed that higher levels of electrical power can be generated at the load resistance using this doping level.

The same set of simulation tests have been performed on the thermoelectric couple and ceramic plate model shown earlier in Fig. 6. If the top of the device, where the thermal contact 'Ceramic top' is located, is set to 301 Kelvin, and the thermal contact 'Ceramic bottom' is maintained at 300 Kelvin, the lattice temperature gradient shown in Fig. 12 is obtained, and appears less pronounced than observed earlier in Fig. 8. The ceramic plates absorb some of the applied temperature gradient, and the temperature gradient within the thermoelectric pellets is now more uniform than before. The electrical power generated at the load under these test conditions is shown in Fig. 13.

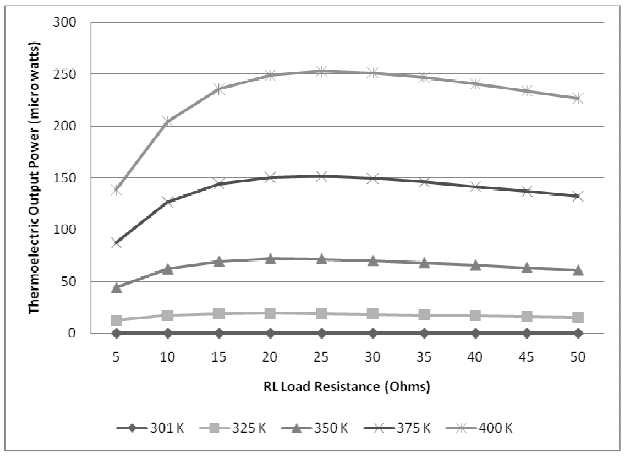

Fig. 11. The electrical power generated at the load resistor (RL) with different temperature settings applied to the thermal contact connected to Copper 1, and a doping level of $1e^{+}16cm^{-3}$ for both P-type and N-type pellets

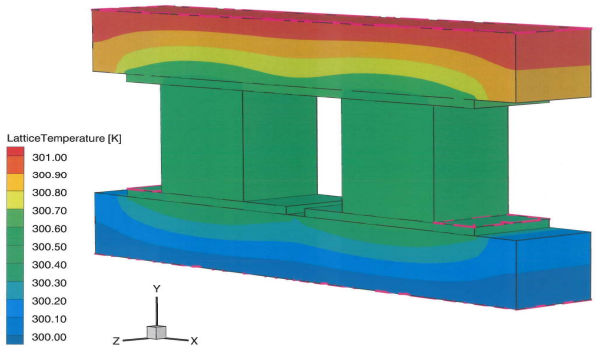

Fig. 12. The lattice temperature for a single thermoelectric couple with ceramic plates, and an applied 1 Kelvin temperature gradient between both sides of the device

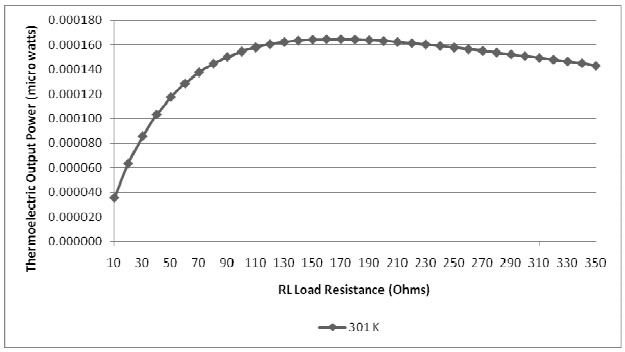

Fig. 13. The electrical power generated at the load resistor (RL) for a single thermoelectric couple with ceramic plates, and a temperature gradient of 1 Kelvin between both sides of the device

As the thermoelectric couple is now at a more uniform temperature, the electrical power generated at the load has been reduced when compared to the previous test without the two ceramic plates. However, the ceramic plates are necessary in practical thermoelectric devices in order to create electrical isolation and provide a foundation to mount the thermoelectric couple. Optimising the material properties of the Ceramic used in the construction of the outer plates, by increasing their thermal conductivity, should improve the electrical power generated by the thermoelectric couple.

It should be noted that the 3D simulation results presented in this paper confirm the 2D TCAD simulation results obtained in previous simulation experiments and published in [7].

8. Conclusions

The 3D simulation of a thermoelectric couple in TCAD has been successfully achieved, and the preliminary simulation results obtained demonstrate the basic principle of thermoelectric power generation. The simulation results appear to be in agreement with basic thermoelectric theory, and the use of Silicon as the base material is sufficient to demonstrate the basic concepts. The TCAD thermoelectric couple simulation model can be used for further analysis into thermoelectric effects, material structure and technology.

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