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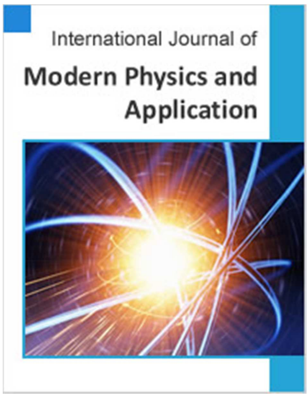

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Thermoelectrically Modeling in Unidirectional Carbon nFiber (UCnF) Reinforced Shape Memory Polymers-(SMPs) Nanostrip Multilayers on the Turbochargers

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Abstract
Shape memory polymers are a special type of polymer, which can recover the permanent shape upon the application of external stimulus. The main advantage of shape memory polymer the ability of recovering a large amount of strain (usually >400%) in comparison to shape memory alloys (SMP) (up to 15%) and shape memory ceramics (2 - 3%) [3, 7, 15]. The material used in this research is Shape Memory Polymer due to its excellent shape recoverability. Before going into the details of the various topics of my work some of the basic features of SMP are discussed first.

1. Introduction

Thermoelectric material converts a difference in temperature to an electric potential or, conversely, anapplied voltage to a difference in temperatureThis phenomenon has made these materials attractive fortheir potential in applications extending from microprocessor cooling to turbocharger &power industry.

Shape Memory Polymers-(SMPs), represent co-polymers which generally the structure consists of twotype of components(figure.1). One component, like nanostrip multilayers, with the higher glass transitionor melting temperature, represent the hard component. This hard component (elastomer) represent themain element of SMPs, which improve the tribological (wearing resistance) properties and provides themechanical strengthof SMPs at high temperature, T_{trans}, where the soft component (thermoplast), whichstabilizes the hard component at low temperature loosesits strength.

Thermoelectric phenomena provide the direct conversion of heat into electricity or electricity into heat, the phenomena are described by three related mechanisms: the Seebeck, Peltier and Thomson effects.

The main objective is to realize pseudo-composite material: Unidirectional Carbon nFiber (UCnF) reinforced shape memory polymers-(SMPs) nanostrip multilayers material -*Vyborcntmat-SMP(VycnT).* It is a challenge for new generation of turbochargers to limit diesel-cars exhaust hot and dangerous gases and protect life and the environment.

To determine the shape memory phenomena mechanical programming cycle has been done on the specimen and the Figure 1.The important processes are described below:

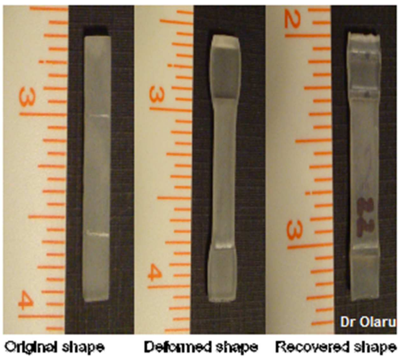


Figure 1. *Thermally driven shape memory cycle of SMP-Vyborcntmat-SMP(VycnT).*

- The specimen is heated to 100°C which is above the glass transition temperature, Tg = X°C, [2, 13, 18];
- At 100°C the specimen has been given a 50% tensile deform. by applying a tensile force on it.
- After the deformation the temperature of the sample has been cooled below the room temperature while maintaining the load on the specimen turbocharger.
- At temperature below the glass transition temperature, the load is removed and the specimen is removed from the fixture. *The resulting shape is called the deformed or temporary shape*.In this condition, the length of the sample has been measured, [4, 11, 17].
- Then it is heated again to 100°C, which is above the glass transition temperature, and no-constraint was imposed on the specimen to recover the original shape.
- Finally, it is cooled to room temperature and the length of the sample has been measuredfrom which the shape memory property of the sample has been calculated.

2. Modeling Catalyst Components in Matlab

To satisfy emissions regulations, a complete aftertreatment system for a diesel engine must remove carbon monoxide, unreactedhydrocarbons, nitrogen oxides (NO_X), and particulate matter. As a result, a complete *Johnson Matthey* aftertreatment system comprisesa diesel oxidation catalyst (DOC), a diesel particulate filter (DPF), an ammonia selective catalytic reduction (NH_3 SCR) catalyst, and anammonia slip catalyst (ASC), [5, 10].

We created MATLAB models for each of these components. The models capture a complex combination of interrelated physical processes and kinetics. The physical processes include gas flows, as well as heat and mass transfer within the catalyst. The kinetics describe the rate at which chemical reactions take place, and show how the rate varies according to temperature and gas composition.

To develop a catalyst model we start with equations that describe the physics of the system, including energy and mass balances for the gas and solid (catalyst) phases, together with equations describing the heat and mass transport between these phases. We then run experiments in the lab that enable us to accurately measure the catalyst's output while precisely controlling input and catalyst parameters, [12, 14].

For example, the method for measure carbon monoxide conversion as a function of temperature for various gas mixtures.

We obtain data for the feed block by capturing engine exhaust data from a real diesel engine as it executes the drive cycle (fig. 2)

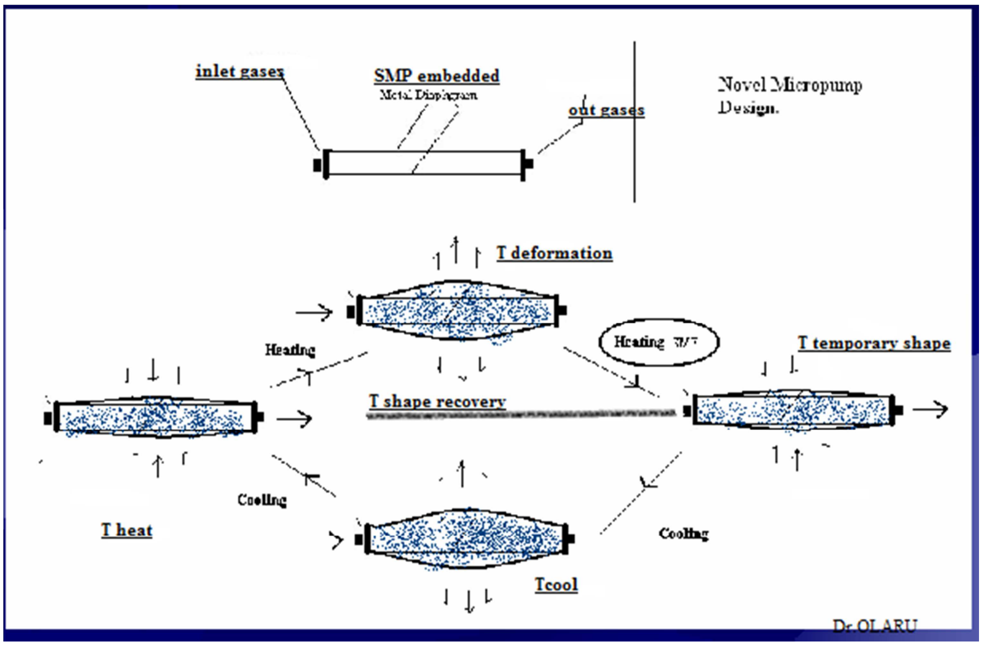


Figure 2. *The diaphragms will bulge out due to initial heating and inlet valve will operate during this period. As temperature increases the shape memory polymer effect will come into picture and this will create stress within the SMP that will drive the diaphragms back to the original positions.*

3. Effect of Frequency on Glass Transition Temperature

The effect of the frequency of the ambient DMA scan of untreated SMP on the position of tan x peak is shown in figures 3, 4 and 5. There is a shift in the tan x peak to a higher temperature with the increase of frequency of the scan. The overall trend is the same, i.e., the glass transition temperature increases with the increase of frequency, [6, 9]. This effect is expected since the glass transition phenomena of SMP resulted from the slippage or rearrangement of the polymeric chain. For the rearrangement of the polymeric chain to occur, a certain amount of heat-energy is required from exhaust turbocompresor. At higher frequency the molecular segments does not get enough time for rearrangement at a certain energy level. As a result, the large-scale molecular motions begin at a higher temperature.

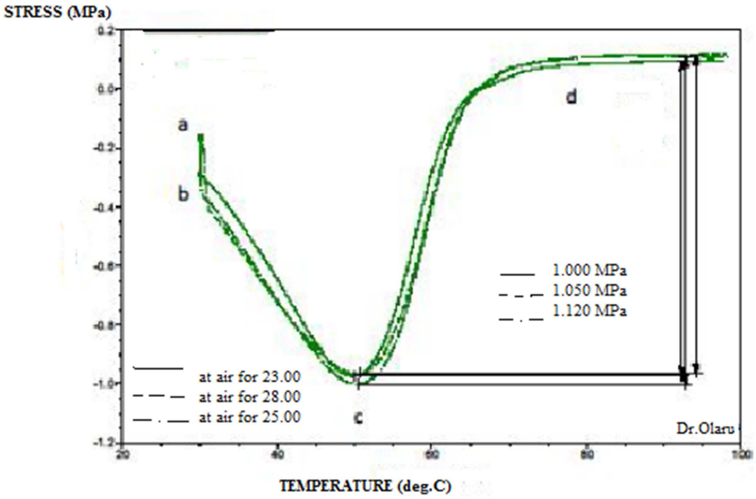


Figure 3. Recovery force curve of shape memory polymer.

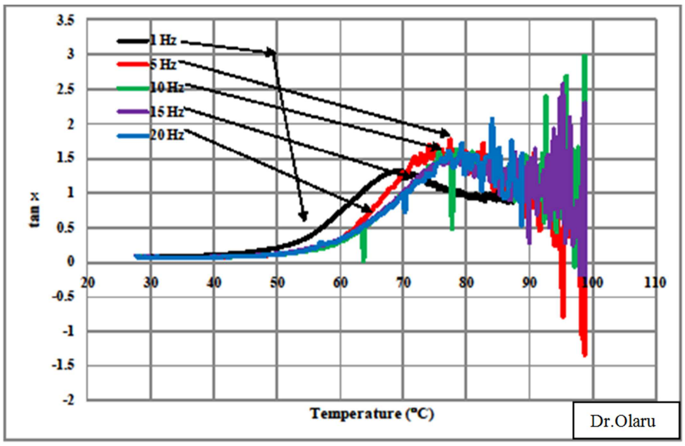


Figure 4. Effect of electric frequency on the glass transition temperature of the SMP.

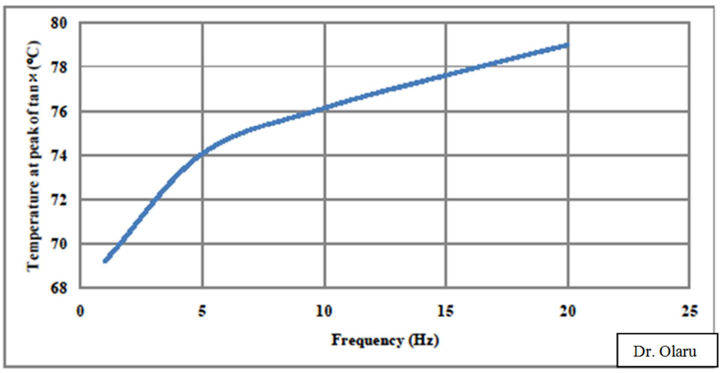


Figure 5. Temperature at the peak of tan x of SMP as a function of electric frequency.

4. Thermoelectric Effect

Thermoelectric phenomena provide the direct method of conversion the heat into electricity or electricity into heat, the phenomena is described by three related mechanisms: the Seebeck, Peltier and Thomson effects.

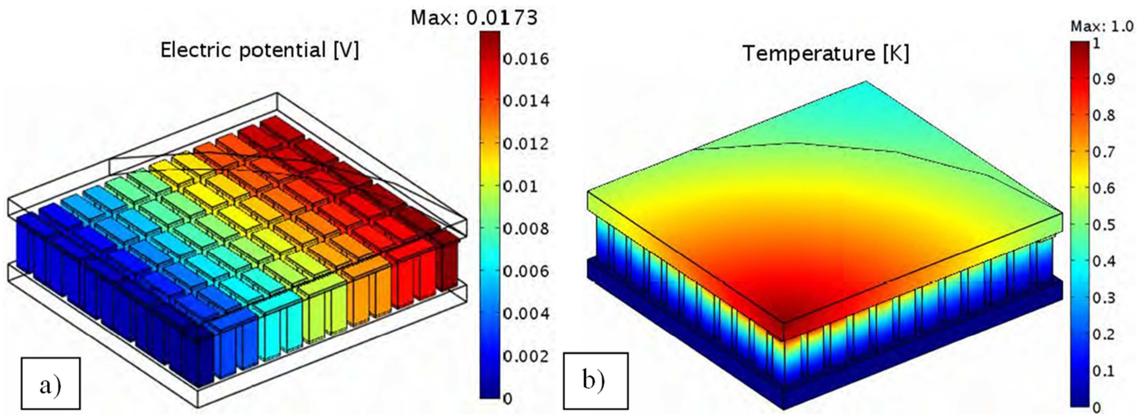
The Seebeck effect describes the conversion of temperature differences directly into electricity; at the atomic scale, an applied temperature gradient causes charged carriers in the material to diffuse from the hot side to the cold side generating a current flow.

The Peltier effect describes the production of heat at an electrified junction of two different materials, the forced flow of charged carriers creates a temperature difference.

The Thomson effect describes the heating or cooling of a current carrying conductor in the presence of a temperature gradient. To analyze these phenomena accurately the thermoelectric field equations have to be solved.

The Seebeck coefficient, *S*, measures the magnitude of an induced thermoelectric voltage in response to a temperature difference across that material, and the entropy per charge carrier in the material. An applied temperature difference causes charged carriers in the material to diffuse from the hot side to the cold side. Mobile charged carriers migrating to the cold side leave behind their oppositely charged nuclei at the hot side thus giving rise to a thermoelectric voltage, [1, 8].Since a separation of charges creates an electric potential, the buildup of charged carriers on the cold side eventually ceases at some maximumvalue. The material's temperature and structure influence *S*; CnF (carbon nanofiber) hasgood Seebeck coefficients whereas semiconductors can be doped to tailor the behavior and increase the Seebeck coefficient [16].

5. Results - Laboratory Works



Figures 6. *Electric potential for a thermoelectric module made up of an array of UCnF & SMP (VycnT) pseudo-composite due to imposition of a non uniform temperature distribution: Seebeck effect.*

Table 1. *Typically material properties for thermoelectric applications.*

Parameters	UCnF & VycnT	Copper electrode
Seebeck coefficient, V/K	200x 10^{-6}	3.8x 10^{-6}
Electrical conductivity, S/m	1.1x 10^{-5}	6x 10^{7}
Thermal conductivity, W/m.K	1.7	400
Heat capacity, J/kg.K	554	385
Density, g/cm^3	Bulk: 0.2-0.4	8800

6. Discussions

1. Control over the orientation or arrangement of a nanostructure can provide advantages and additional leverage for certain applications; Example: Oriented 1D: Unidirectional Carbon nFiber -UCnF (nanostrip multilayers), such as *UcnF&Vyborcntmat-SMP(VycnT)*, can outperform non-oriented counterparts in specific applications. It has been shown that vertically-oriented *VycnT,* or *VycnT* arrays have attractive characteristics as field emission electron sources for devices including flat panel displays [15], gas discharge tubes, and lamps. When an electrical potential is applied between a *VycnT* array and an anode, high local electric fields can be produced due to the very small radius of the *VycnT* tip and the length of the *VycnT,* which causes for electron-noxes to tunnel effect to capture, adsorb and absorb from the Turbine Exhaust Hot GAS majority impurities similar *nanotube tip into the vacuum*.
2. Similarly, when the orientation of *VycnT* on a substrate is changed from being planar or horizontal (randomly oriented or parallel to the substrate surface) to being vertical (perpendicular to the substrate surface), i.e., to form V-O; it is promising to effectively harvest both intrinsic properties of *VycnT*and additional characteristics due to the free standing arrangement;

3. Efficiency of *UcnF&Vyborcntmat-SMP (VycnT)* in reinforcing SMPs polymer strongly depends on the chemical structure of *VycnT* at atomic scale while load transferring from matrix to *VycnTs* through the intermediate phase between *VycnTs* and surrounding SMPs polymer plays a key role at micro-scale.
4. However, resolving such issues is a matter of time as processing and characterization technologies are being advanced rapidly. On the fabrication side, *for example*, investigators developed a new synthetic approach that can afford a flawless *VycnT with* control of its structure and length.
5. Among those atomistic simulation methods, molecular dynamics (MD) has been acknowledged to be a powerful method for providing a better understanding of the role of atomistic structures of materials at the macroscopic scale.

7. Conclusions

This synthesis-work has demonstrated the implementation of the thermoelectric field equations for the Peltier-Seebeck effects in COMSOL Multiphysics. Examples of the application of the implantation have been provided for both the conversion of temperature differences directly into electricity and the generation of heat due to the imposition of an electric potential.

1. COMSOL Multiphysics can be used to model the electrical conductivity of unidirectional carbon nfiber (UCnF) reinforced SMPs (*VycnT) like pseudo-composites*.
2. Conductivity models were produced for above and below the percolation threshold.
3. The percolation model was validated through agreement with experimentally determined contact resistance between two fibers.
4. Electrical conductivity was modeled across the entire UCnF loading range.
5. These basic models were scaled to a more typical industrial pseudo-composite consisting of multiple plies with different contact configurations with Advantages vs. Limitations:

A. Advantages:

a. Thermal performance was validated and it is in good agreement with experiments- FACVD (*plasma-free vacuum technology*) capable of producing UCnF suitable for advanced interconnects;

b. Determined sticking coefficient of polymer-shape memory polymers-(SMPs) nanostrip, (μ=~ 0.035) and effective activation energy (~ 4.23 J/mol) for “FACVD mode polymerization”

c. In virtual model, the film properties and complex processes can be adjusted simply by input parameters - computational DOE and hypothesis verification;

d. Peltier/Seebeck terms implemented using weak form methods;

e. Fully coupled temperature dependent material properties;

f. Predict effect of imposed thermal gradients;

g. Predict effect of electric current flow;

B. Limitations:

1. The most material properties, controlling the microstructure are key to optimizing thermoelectric performance. Two specific areas being researched to improve efficiency are crystallographic texture and the arrangement and types of grain boundaries.

2. It gives you more miles per gallon when compared to petrol engines and limit pollution.

3. The logic there is burning and exhausts less poison gas (ex: CO_2, CO, Nox, etc.)

4. So, when it comes to global warming, diesel emissions are possibly “greener” than fuel / petrol.

5. However, diesel engines produce more nitrogen oxides and particulate matter than petrol engines. It is the emission of nitrogen oxides and particulate matter, and the associated formation of secondary pollution, that leads to air quality problems in towns and cities.

6. So, because of air quality and health impacts I’d say that, overall, diesel engines aren’t greener, yet?

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