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 is 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%).

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.

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 andtheenvironment

Keywords: Shape memory polymer, nanofiber, nanostrip, thermoelectric, modeling

1. INTRODUCTION

Thermoelectric material converts a difference in temperature to an electric potential or, conversely, an applied voltage to a difference in temperature This phenomenon has made these materials attractive for their potential in applications extending from microprocessor cooling to turbocharger & power industry.Shape Memory Polymers-(SMPs), represent co-polymers which generally the structure consists of two type of components (**Figure 1**). One component,like nanostrip multilayers, with the higher glass transition or melting temperature, represent the hard component. This hard component (elastomer) represent the main element of SMPs, which improve the tribological (wearing resistance) properties and provides the mechanical strength of SMPs at high temperature, $\mathbf{T_{trans}}$, where the soft component (thermoplast), which stabilizes the hard component at low temperature looses its strength.

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- 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 onthespecimen 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 ofthe sample has been measured, [4,11].
- Then it is heated again to 100 °C, which is above the glass transition temperature, and no-constraint was imposedonthe specimen to recover the original shape.
- Finally, it is cooled to room temperature and the length of the sample has been measured from which the shape memory property of the sample has been calculated.

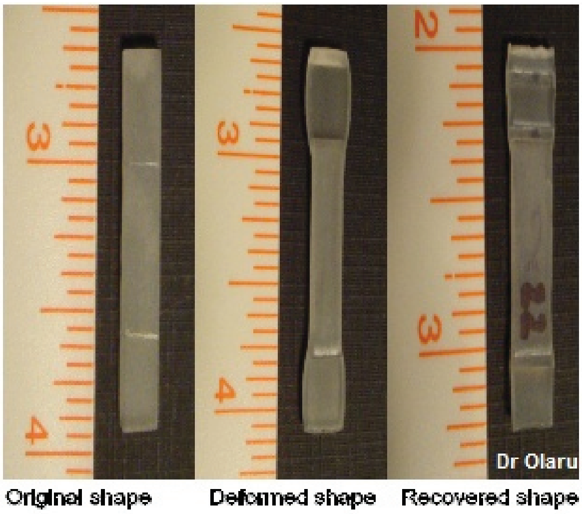

Figure 1 Thermally driven shape memory cycle of SMP-Vyborcntmat-SMP(VycnT)-The specimen is heated to 100ºC which is above the glass transition temperature, Tg = XºC,[2, 13]

2. MODELING CATALYST COMPONENTS IN MATLAB

To satisfy emissions regulations, a complete aftertreatment system for a diesel engine must remove carbon monoxide, unreacted hydrocarbons, nitrogen oxides (NO_X), and particulate matter. As a result, a complete *Johnson Matthey* aftertreatment system comprises a diesel oxidation catalyst (DOC), a diesel particulate filter (DPF), an ammonia selective catalytic reduction (NH_3 SCR) catalyst, and an ammonia 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.

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 2, 3** and **4a, 4b**. 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 re-arrangement 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.

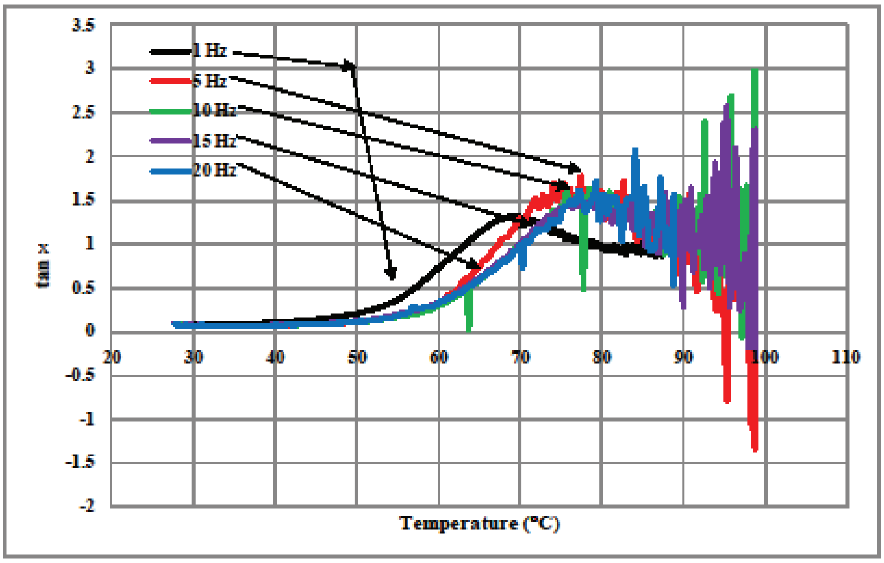

Figure 2 Effect of the electric frequency on the glass transition temperature of the SMP

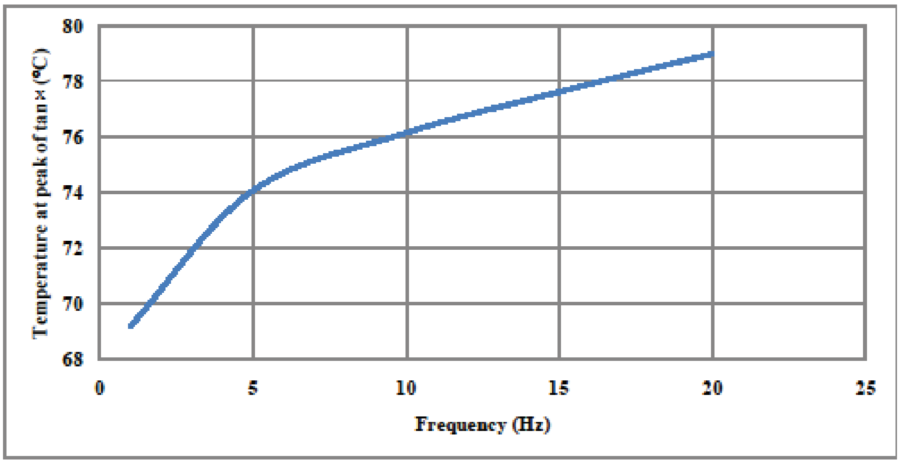

Figure 3 Temperature at the peak of ***tan x*** of SMP as a function of electric frequency

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 maximum value.The material's temperature and structure influence ***S***; **CnF (carbon nanofiber) has good Seebeck coefficients whereas semiconductors can be doped to tailor the behavior and increase the Seebeck coefficient** [15].

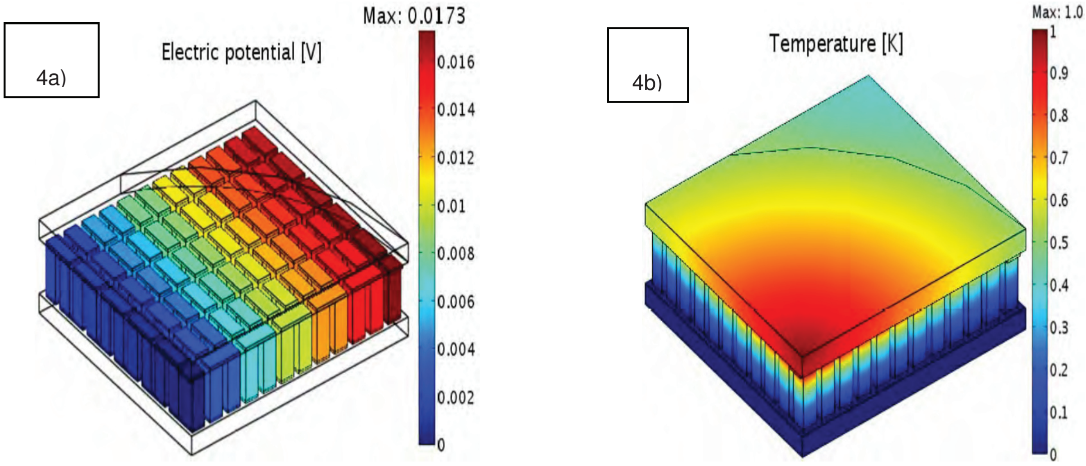

Table 1.Typically material properties for thermoelectric applications

Parameters	*UCnF & VycnT*	*Copper electrode*
Seebeck coefficient, V/K	$200x\ 10^{-6}$	$3.8x\ 10^{-6}$
Electrical conductivity, S/m	$1.1x\ 10^{-3}$	$6x\ 10^{7}$
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

Figures 4a, 4b Electric potential, temperature evolution and **table 1** of the material properties 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***

5. 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.

REFERENCES

[1] KCA Crane, Laser-Induced Ablation of Fibre/Epoxy Composites, *Journal of Applied*, *Physics,* **14,** 1981.

[2] KT Voisey, Fibre Swelling During Laser Drilling of Carbon Fiber Composites, *Optics Lasers Engineering,* **44,** 2006.

[3] CT Pan, Evaluation of Anisotropic Thermal Conductivity for Unidirectional FRP in laser Machining, *Composites Part A*, **32**, 2001.

[4] CT Pan, Prediction of Extent of HAZ in Laser Grooving of Unidirectional Fiber Reinforced Plastics, *Journal of EngineeringMaterials and Technology,* **120**, 1998.

[5] E Uhlmann, The Extent of Laser Induced Thermal Damage of UD and Crossply Composite Laminates, *International Journalof Machine Tools & Manufacture*, **39**, 1999.

[6] WSO Rodden, A Comprehensive Study of the Long Pulse Nd:YAG Laser Drilling of Multi-Layer CarbonFiber Composites, *Optics Communications,* **210,** 2002.

[7] MD Islam, Thermal Conductivity of Fiber Reinforced Composites by the FEM, *Journal of Composite Materials*, **33,** 1999.

[8] CF Cheng, Application of a 3-D Heat Flow Model to Treat Laser Drilling of Carbon Fiber Composites, *Acta Metallurgica,* 1998.

[9] LN Nikitin, Calculation of the Temperature of Polymer or Composite Surfaces Placed in an Infrared Laser Field, *Mechanics ofComposite Materials*, **31**, 1995.

[10] Toshiki Hirogaki, Prediction of Damage Width in Laser Drilling of Printed Wiring Board using FEM, *ICCM Proceedings*, 1997.

[11] Robert Cozzens, High Energy Laser Interactions with Organic Matrix Composites, *N. R.. Lab.*, 2007.

[12] Solid State laser Technology Maturation program *WAREX, ONR, 2012*.

[13] Christopher Lloyd, Ablative Polymeric Materials for Near-Infrared High-Energy Laser Beam Diagnostics,*Journal of Directed Energy*, **3,** 2009.

[14] M Dell'erba, An Experimental Study on Laser Drilling and Cutting of Composite.

[15] The Boeing Company. *787 Advanced Composite Design*. 2008-2013