Chapter 22
Using Theoretical and Computational Models to Understand How Metals Function as Temperature Sensors

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ABSTRACT
Electrical conductivity is a basic property of materials that determines how well the material conducts electricity. However, models are needed that help explain how conductors function as their size and temperature changes. This research demonstrates and explains how important atomic motion is in understanding electrical conductivity for conductors (and thus the ability of metals to function as temperature sensors). A derivation is performed (on an atomic level) that provides a theoretical relationship between electrical resistivity, temperature, and material thickness. Subsequently, computational models are used to determine the optimal parameters for the theoretical models as well as the conditions under which they are accurate. Comparisons are performed using experimental data showing that the models are valid and accurate.

INTRODUCTION
Resistance temperature detectors (RTDs) are metals that function as temperature sensors. These devices have a well known response between their electrical resistance and temperature. As a result, these materials have found much success as temperature detectors or temperature sensors. Because temperature measurements are necessary in many diverse fields, RTDs currently find applications in biology and medicine (Cavallini 2012, Liu 2014, Yi 2014), battery and fuel cell research (Lee 2013, Lee 2014, Wang 2014a), aeronautics (Daniels 2012, Miyakawa 2012), materials science (Abeykoon 2012, Zhang 2013, Using Theoretical and Computational Models to Understand How Metals Function as Temperature Sensors

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Jiang (2014), environmental monitoring (Park 2011, Li 2012, Holstein-Rathlou 2014), food processing (Singh 2012, Ranasinghe 2013), and chemical or gas detection (Chee 2014, Wang 2014b). Reducing the size of RTDs for these applications could affect their response.

A theoretical model has been created to elucidate the mechanisms that affect the electrical resistance of metals or conductors. The core of the model involves the atoms of the crystal lattice and their ability to impede the flow of electrons. The model demonstrates that the flow of electrons in the conductor will be increasingly affected as the temperature increases due to an increase in the obstructed flow path. As a result of this property, metals can be used to monitor temperature (and temperature changes) by measuring their electrical resistance. The theoretical model contains variables for atomic diameter, separation distance, energy associated with the atoms, as well as electron scattering times. When these factors are properly assessed through computational analysis, this model shows that as the vibrations of the atoms in the lattice increase, due to an increase in temperature, the electrical resistivity increases as well. This result clearly demonstrates the temperature sensing property of metals. After the values of the aforementioned variables are properly selected, the model provides data that matches experimental results.

Moreover, since material properties are known to change when a material’s dimensions are diminished to nanoscale levels, the theoretical model was expanded to account for nanoscale effects. After computational analysis is performed on this modified theoretical model, comparisons with experimental data demonstrate that the modified theoretical model is accurate for both bulk and thin film materials. Finally, since electrical current is typically supplied to RTDs in order to measure temperature changes, and since this supplied current will cause Joule heating (and thus elevated temperatures), finite element modeling was used to assess this effect. Analysis shows that reasonable currents can be supplied to the RTD without causing significant measurement error. Since the model is found to be accurate (when analyzing a bulk or thick film conductor at varying temperatures, a thin film conductor at varying temperatures, and a conductor of variable thickness at constant temperature), it provides a useful tool in understanding fundamental electrical properties of conductors.

As a result, the objective of this report is to present a theoretical models relating electrical resistivity to material size and temperature. Subsequently, various computational modeling is used to show that the models are accurate.

BACKGROUND

If only one material property is singled out as the most important in electrical engineering, many would agree that electrical resistivity should be that property. This parameter determines how well the material will conduct electrical current. Everything from microelectronic circuits to electrical power transmission relies on wires and connections that have low resistivity. Since a material’s resistance to current flow is not a static parameter, it is extremely important to understand how and why resistance changes.

In the field of electrical and electronics engineering, one of the important tasks in circuit design is controlling the electrical current and/or power consumption in a circuit. This is accomplished by placing materials of a particular electrical resistance in the proper location in the circuit. The electrical resistance of a material is known to be a function of its dimensions as well as its electrical resistivity (a parameter that depends upon the type of material). Because electrical resistance is known to vary with the dimensions of the material, scientists and engineers often choose to characterize a material by its electrical resistivity and not its resistance.