Y-12

OAK RIDGE Y-12 PLANT

LOCKHEED MARTIN

Project Accomplishment Summary
for
Project Number 92-MULT-021-B2-4A

**MATERIALS BY COMPUTATIONAL DESIGN - HIGH
PERFORMANCE THERMOELECTRIC MATERIALS**

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Project Accomplishment Summary

Title: Materials by Computational Design – High Performance Thermoelectric Materials
DOE TTI Number: 92-MULT-021-B2-4A
CRADA Number: ORNL92-0116
Partner: Marlow Industries, Inc.

Background:

The objective of the project was to utilize advanced computing techniques to guide the development of new material systems that significantly improve the performance of thermoelectric devices for solid state refrigeration. Lockheed Martin Energy Systems, Inc. (LMES) was to develop computational approaches to refine the theory of the thermoelectric effect, establish physical limits, and motivate new materials development. Prior to the project, no major activity in thermoelectric research was visible as an observed limit in experimental data was commonly accepted as a practical limit by the majority of informed opinion in the physics and thermoelectric community. Due to the efforts of the project, new compounds have been isolated which indicates that there is a physical reason to search through the remaining uncharacterized compounds from a top down theoretical approach.

Description

Due to the low efficiency of thermoelectric effects, the use of thermoelectricity has been limited to places where quick heat and/or refrigeration is needed and efficiency is not of utmost importance. The objective of the partnership with Marlow Industries was to use advanced computing techniques to guide the development of new materials that would significantly improve the performance, particularly efficiency, of thermoelectric devices for solid state refrigeration.

LMES scientists in conjunction with scientists from the industrial partner developed computational approaches to refine the theory of thermoelectricity (specifically the Peltier effect), established physical limits, and motivated new materials development. From the computer model, the partnership investigated a wide variety of material systems, which showed promise for new thermoelectric applications. In addition to contributing to the development of computer models, Marlow Industries contributed to the candidate materials selection process and fabricated thermoelectric elements for testing. The testing which was conducted at LMES facilities in Oak Ridge was used to validate the material design models.

By the use of detailed computer simulations, Lockheed Martin Energy Systems investigated a wide variety of materials systems including layered structures and Kondo Alloys, which showed promise for new thermoelectric applications. Based on theoretical guidance from the simulations, LMES synthesized and characterized candidate thermoelectric materials. Marlow Industries participated in the development of computer models, contributed to the candidate materials selection process, and fabricated thermoelectric elements for validation of the materials design models.

Conclusions reached utilizing the computer models developed by this project would have taken 3

to 6 years if only experimental data had been used. Theoretical accomplishments have been published in Physics Review (1994), Proceedings of the National Academy of Sciences (1996), Applied Physics Letters (1994), and the Journal of Applied Physics (1995). The experimental results have been published in Physics Review (1994) and the Journal of Applied Physics (1995).

Because of these efforts, the analysis of the reduced dimensional structures has finally been accepted by the leadership of the superlattice community, as well as the analysis of what the ideal thermoelectric structure should look like.

Benefits To DOE:

Spot thermoelectric refrigeration is of potential use in any machining process where there is a concern with vibration, noise, or a need to avoid possible chemical reactions that would be associated with the introduction of a liquid coolant into the vicinity of the process. For example, at the Y-12 Plant there is a desire to avoid the introduction of liquids into the process chamber for some of the more potentially hazardous processes that must be performed in a dry atmosphere. Thermoelectric refrigeration could also be utilized in other potential specialized refrigeration needs of Defense Programs such as the cooling of noise sensitive electronic systems. The work performed during this CRADA significantly advanced the science of thermoelectric materials and devices, which may be of use in these applications.

Economic Impact:

By the end of this project, the effort of LMES was acknowledged as a leadership effort, of a balanced and highly professional theoretical and experimental scientific effort, an effort which through its pronouncements and publications gave new life to an otherwise dormant field of inquiry at a time when it was strategically important to make a move. Science moves on more than successful applications as the sole measure of achievement, the joint project between Marlow Industries and LMES documents the initiation of a second era in the history of thermoelectric. The numerous papers and comprehensive coverage of the analysis produced in this effort has initiated a large US effort which Marlow Industries Inc. presently perceives will result in a two fold or more increase in the thermoelectric market which Marlow Industries ultimately values at near a billion dollars annually. It is the perception of Marlow Industries that without the efforts put forth in this project, it is highly possible that the Russian and Japanese effort would be taking this new market away from US suppliers.

Project Status:

The project is complete

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Project Examples:

No project examples are available due to the lapse of time since the end of the project and now.

Technology Commercialization:

Prior to full commercialization of this technology, there are still several additional research tasks to complete. Once they are completed, it will assure US firms a leadership position in the thermoelectric field.

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