12:58:17 OCA PAD INITIATION - PROJECT HEADER INFORMATION 08/04/95

Active

Project #: E-27-686 Cost share #: E-27-348 Rev #: 0
Center # : 10/24-6-R8630-0A0 Center shr #: 10/22-1-F8630-0A0 OCA file #:
Work type : RES
Contract#: DMR-9503936 Mod #: Document : GRANT
Prime #: Contract entity: GTRC

Subprojects ? : N CFDA: 47.049
Main project #: PE #: N/A

Project unit: TEXT ENGR Unit code: 02.010.130
Project director(s):
BECKHAM H W TEXT ENGR (404)894-2490

Sponsor/division names: NATL SCIENCE FOUNDATION / GENERAL
Sponsor/division codes: 107 / 000

Award period: 950815 to 960731 (performance) 961031 (reports)

Sponsor amount	New this change	Total to date
Contract value	337,140.00	337,140.00
Funded	337,140.00	337,140.00
Cost sharing amount		224,760.00

Does subcontracting plan apply ?: N

Title: ACQUISITION OF A 400-MHZ MULTINUCLEAR SOLID-STATE NMR SPECTROMETER WITH.....

PROJECT ADMINISTRATION DATA

OCA contact: Jacquelyn L. Bendall 894-4820

Sponsor technical contact

LORRETTA J. INGLEHART
(703)306-1817

NATIONAL SCIENCE FOUNDATION
4201 WILSON BLVD.
ARLINGTON,VA 22230

Sponsor issuing office

RONALD T. BARON
(703)306-1213

NATIONAL SCIENCE FOUNDATION
4201 WILSON BLVD.
ARLINGTON, VA 22230

Security class (U,C,S,TS) : U ONR resident rep. is ACO (Y/N): N
Defense priority rating : N/A NSF supplemental sheet
Equipment title vests with: Sponsor GIT X

Administrative comments -
INITIATION OF PROJECT. GIT AGREES TO PROVIDE COST SHARING IN THE AMOUNT OF $224,760 AS A CONDITION OF THIS AWARD.

4

GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION

NOTICE OF PROJECT CLOSEOUT

Closeout Notice Date 12/06/96

Project No. E-27-686_____ Center No. 10/24-6-R8630-0A0_

Project Director BECKHAM H W_____ School/Lab TEXT ENGR_____

Sponsor NATL SCIENCE FOUNDATION/GENERAL_____

Contract/Grant No. DMR-9503936_____ Contract Entity GTRC

Prime Contract No. _____

Title ACQUISITION OF A 400-MHZ MULTINUCLEAR SOLID-STATE NMR SPECTROMETER WITH..

Effective Completion Date 960731 (Performance) 961031 (Reports)

Closeout Actions Required:	Y/N	Date Submitted
Final Invoice or Copy of Final Invoice	N	_____
Final Report of Inventions and/or Subcontracts	N	_____
Government Property Inventory & Related Certificate	N	_____
Classified Material Certificate	N	_____
Release and Assignment	N	_____
Other _____	N	_____

Comments_____
LETTER OF CREDIT APPLIES. 98A SATISFIES PATENT REPORT._____

Subproject Under Main Project No. _____

Continues Project No. _____

Distribution Required:

Project Director	Y
Administrative Network Representative	Y
GTRI Accounting/Grants and Contracts	Y
Procurement/Supply Services	Y
Research Property Managment	Y
Research Security Services	N
Reports Coordinator (OCA)	Y
GTRC	Y
Project File	Y
Other _____	N
_____	N

E-27-686 #1

OMB Number 345-0058

NATIONAL SCIENCE FOUNDATION
4201 Wilson Blvd.,
Arlington, VA 22230

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POSTAGE & FEES PAID
National Science Foundation
Permit No. G-69

PI/PD Name and Address

Haskell W. Beckham
Department of Textile & Fiber Eng.
GA Tech Res Corp - GIT
Atlanta GA 30332-0295

NATIONAL SCIENCE FOUNDATION
FINAL PROJECT REPORT

PART I - PROJECT IDENTIFICATION INFORMATION

1. Program Official/Org. Lorretta J. Inglehart - DMR

2. Program Name NATIONAL FACILITIES AND INSTRUMENTATION

3. Award Dates (MM/YY) From: 08/95 To: 07/96

4. Institution and Address
GA Tech Res Corp - GIT
Administration Building
Atlanta GA 30332

5. Award Number 9503936

6. Project Title
Acquisition of a 400-MHz Multinuclear Solid-State NMR Spectrometer with Wide-Bore 9.4-Tesla Magnet

** You are encouraged to submit your Final Project Report electronically through the NSF FastLane home page (www.fastlane.nsf.gov). **

This Packet Contains
NSF Form 98A
And 1 Return Envelope

NSF Grant Conditions (Article 17, GC-1, and Article 9, FDP-11) require submission of a Final Project Report (NSF Form 98A) to the NSF program officer no later than 90 days alter the expiration of the award. Final Project Reports for expired awards must be received before new awards can be made (NSF Grants Policy Manual Section 677).

Below, or on a separate page attached to this form, provide a summary of the completed projects and technical information. Be sure to include your name and award number on each separate page. See below for more instructions.

PART II - SUMMARY OF COMPLETED PROJECT (for public use)

The summary (about 200 words) must be self-contained and intelligible to a scientifically literate reader. Without restating the project title, it should begin with a topic sentence stating the project's major thesis. The summary should include, if pertinent to the project being described, the following items:

- The primary objectives and scope of the project
- The techniques or approaches used only to the degree necessary for comprehension
- The findings and implications stated as concisely and informatively as possible

PART III - TECHNICAL INFORMATION (for program management use)

List references to publications resulting from this award and briefly describe primary data, samples, physical collections, inventions, software, etc. created or gathered in the course of the research and, if appropriate, how they are being made available to the research community. Provide the NSF Invention Disclosure number for any invention.

I certify to the best of my knowledge (1) the statements herein (excluding scientific hypotheses and scientific opinion) are true and complete, and (2) the text and graphics in this report as well as any accompanying publications or other documents, unless otherwise indicated, are the original work of the signatories or of individuals working under their supervision. I understand that willfully making a false statement or concealing a material fact in this report or any other communication submitted to NSF is a criminal offense (U.S. Code, Title 18, Section 1001).

[redacted]	11-23-96
Principal Investigator/Project Director Signature	**Date**

IMPORTANT:
MAILING INSTRUCTIONS
Return this *entire* packet plus all attachments in the envelope attached to the back of this form. Please copy the information from Part I, Block I to the *Attention block* on the envelope.

Acquisition of a 400-MHz Multinuclear Solid-State NMR Spectrometer with Wide-Bore 9.4-Tesla Magnet

Grant No. DMR-9503936

Final Report

Haskell W. Beckham

School of Textile and Fiber Engineering
Georgia Institute of Technology
Atlanta, GA 30332-0295

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404-894-4198
fax:404-894-9766

Summary

After critical examination of the instrumentation provided by the three major NMR spectrometer manufacturers, a decision was made to go with Bruker instruments as the vendor. With additional matching funds, and by including some used equipment in the total package, two complete multinuclear solid-state NMR spectrometers with wide-bore magnets were acquired. The 400-MHz system is equipped with a 4-mm CP/MAS probe, and a microimaging accessory which includes the gradient amplifiers and an imaging probe. A 300-MHz system is equipped with a 7-mm CP/MAS probe, a double-resonance static probe, and a single-resonance wideline probe. Both systems have been installed and most specifications have been met by the manufacturer. They reside in a renovated facility that is the core of the newly established Georgia Tech NMR Center. The Center operates as a campus-wide multiuser facility, and thereby provides access to solid-state NMR and imaging capabilities that were previously nonexistent at Georgia Tech. These techniques are already figuring prominently in the research efforts of a number of groups working in the area of materials synthesis and analysis.

Technical Information

Much work was done to extend the NSF funding. The original proposal requested $337,140 which was matched with $224,760 (40%) from Georgia Tech. After the proposal was funded, an additional $66,261 was directly included for the purchase of NMR spectrometers. In addition, indirect funding totaling about $115,000 was spent for facility renovation, facility furnishings, and peripheral computing/storage/printing equipment. If this indirect funding is included, then the Georgia Tech matching contribution was 55%. The result is an excellent campus-centralized NMR Center. The attached announcement was recently sent out to the Georgia Tech campus. In addition to solids and imaging spectrometers, the Center includes a whole array of spectrometers for liquid samples as well.

As predicted by one of the reviewers, seriously considering three major spectrometer manufacturers enabled us to get an excellent deal. Bruker was chosen primarily because they were deemed most able to supply both solids and imaging on spectrometers to be used by a wide variety of users. Their windows/menu-driven software is currently the best in the business because it is user-friendly yet extremely powerful. Its user-friendliness lies in the fact that it resembles graphical user interfaces seen on desktop personal computers. Bruker has invoiced Georgia Tech for some 80% of the total package

price, and will receive the final 20% as soon as all specifications have been met. This should happen within the next two weeks.

To date, the two solids spectrometers have been used by over 15 different researchers. This number is expected to grow, of course, as the materials research communities at Georgia Tech, Clark-Atlanta, and other Atlanta-area universities (e.g., Emory University) discover what solid-state NMR can enable them to do. Work performed at the NMR Center has already been submitted for publication in the ACS Polymer Preprints for the spring '97 ACS meeting in San Francisco:

"The Mechanical α Relaxation in Poly(ε-caprolactone) Investigated by Solid-State NMR Spectroscopy" Karthik Nagapudi and Haskell W. Beckham, *Polymer Education and Research Center, Georgia Institute of Technology*, Atlanta, GA 30332-0295.

"Synthesis and Dynamic Mechanical Properties of Aliphatic Polyurethane Rotaxanes" Jason Hunt, Karthik Nagapudi, and Haskell W. Beckham, *Polymer Education and Research Center, Georgia Institute of Technology*, Atlanta, GA 30332-0295.

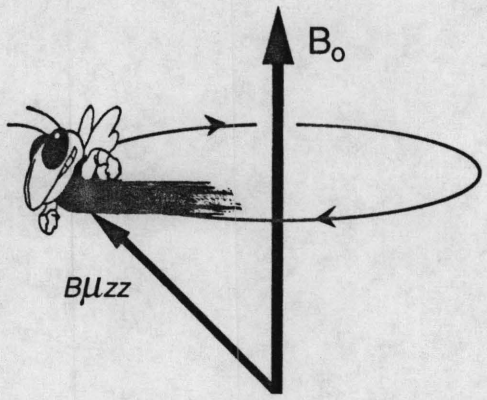
The imaging spectrometer is the only one of its kind intended primarily for imaging fluids in engineered fibrous substrates. A number of funded research projects depend on access to these spectrometers. Some these include the following:

"Structure/*Mobility*/Property Relationships in Polymers and Engineered Fibrous Substrates"
National Science Foundation, Career Award (DMR-9502246)
$312,500. 7/95 to 6/00

"Component-Based Mobility-Directed Polymer Synthesis"
National Science Foundation, Research Initiation Award (CMS-9412294)
$89,952. 7/94 to 6/97

"High-Yield Membrane Reactors"
NSF/EPA Partnership for Environmental Research
$270,000. 7/95 to 6/98 with Mary Rezac, CHE

"The Effect of Comonomers on Chain Dynamics of PET by NMR Spectroscopy"
Hoechst-Celanese Seed Grant Program
$22,500 1/96 to 12/96 with David Collard, CH



Georgia Tech NMR Center

NEW NUCLEAR MAGNETIC RESONANCE CENTER IS OPEN!

Facility Description

The Georgia Tech NMR Center has been established as a campus-wide multiuser facility to support a wide variety of materials and chemical synthesis and characterization. Located in Boggs B-46 and B-47, the Center houses the following nuclear magnetic resonance instrumentation:

500-MHz Bruker DRX for high-resolution liquids, intended for multidimensional spectral acquisition of complex samples. Used for ^{1}H NMR when sensitivity or spectral dispersion are important. Includes triple resonance and pulsed gradient capabilities.

400-MHz Bruker DSX for solids and micro-imaging, high-resolution spectra of solids containing quadrupolar nuclei, and NMR imaging studies of liquids in solid substrates.

300-MHz Bruker DSX for solids, high-resolution solids acquisition, wideline NMR studies of molecular dynamics and orientation.

400-MHz Bruker AMX for high-resolution liquids, totally multinuclear but intended for nuclei other than ^{1}H and ^{13}C. Equipped with a 10-mm probe for samples where solubility is limited. An automatic sample changer allows for overnight acquisitions of multiple samples.

300-MHz Varian Gemini for routine ^{1}H and ^{13}C liquids acquisitions. This spectrometer supports campus-wide research involving chemical syntheses. The system is being upgraded.

The four Bruker spectrometers are completely multinuclear and include variable temperature capabilities. As of 8/26/96, all instruments are operational with the exception of the DSX 400.

Management

The Center will be managed by Leslie T. Gelbaum (894-4079, 894-1827, lg2@prism.gatech.edu) with the assistance of a Users Advisory Group. The Users Advisory Group will consist of primary users, appointed by the Dean of the College of Sciences and representing each unit in which users reside. The Center Manager will be responsible for scheduling and maintenance of the spectrometers, user training, and for providing NMR spectroscopy services. The Users Advisory Group will assist the Center Manager in establishment and evolution of Center policies and operation. Current members of the Users Advisory Group include: Mike Perdue (EAS), Mark

White (CHE), Rob Whetten (PHYS), Leon Zalkow (CH), Will Rees (MSE), Bob Schwerzel (GTRI), Kent Barefield (COS, ex-officio) and Haskell Beckham (TFE, chair).

Scheduling

The instruments will be divided up into two scheduling groups:

(1) Time on the DRX 500, DSX 400, DSX 300, and AMX 400 will be assigned at weekly booking meetings in order to facilitate equal and fair access. Initially, these meetings will take place at 12 noon on Thursdays for time beginning the following Monday morning. One representative from each research group should be present to request time for all members of that group. Request conflicts will be arbitrated by the Center manager. Whatever time remains after these meetings can be had on a first-come, first-served basis. If one cannot be present at these meetings, requests can be submitted via e-mail (lg2@prism.gatech.edu), but must be received before noon on Thursdays. Booking meetings begin 8/29/96.

(2) The Varian Gemini 300 will remain an open access instrument to all individuals who have been trained. Access is first-come, first-served on a weekly time sheet that is put up every Monday morning. Internet sign-up software is currently being evaluated.

The Center Manager reserves time for user training, instrument maintenance, and operator-acquired spectra. One SGI work station exists in the Center for dedicated offline data processing.

Costs

The NMR Center will operate as a cost center. Charges will be made directly to Georgia Tech accounts which have already been created. Funds collected will be used for the daily operation of the center. Hourly fees are set as follows:

spectrometer usage	$7.	9 am to 6 pm on weekdays
	$4.	6 pm to 9 am on weekdays weekends and holidays
operator-assisted	$20.	including user training
non-academic users	$71.	

Time between quarters is not considered holidays. Operator-assisted charges include time for set-up and instrument time. This charge structure is based on current and projected usage of the spectrometers. It will be periodically updated as actual usage data are collected. In order to encourage the development of a users' facility, the operator-assisted rate will possibly increase.

Funding for the Georgia Tech NMR Center has come from a variety of sources:

National Science Foundation
College of Sciences
School of Textile and Fiber Engineering
Molecular Design Institute
State of Georgia
College of Engineering
School of Chemistry and Biochemistry
Polymer Education and Research Center

PART IV -- FINAL PROJECT REPORT -- SUMMARY DATA ON PROJECT PERSONNEL

(To be submitted to cognizant Program Officer upon completion of project)

The data requested below are important for the development of a statistical profile on the personnel supported by Federal grants. The information on this part is solicited in resonse to Public Law 99-383 and 42 USC 1885C. All information provided will be treated as confidential and will be safeguarded in accordance with the provisions of the Privacy Act of 1974. You should submit a single copy of this part with each final project report. However, submission of the requested information is not mandatory and is not a precondition of future award(s). Check the "Decline to Provide Information" box below if you do not wish to provide the nformation.

Please enter the numbers of individuals supported under this grant.
Do not enter information for individuals working less than 40 hours in any calendar year.

	Senior Staff		Post-Doctorals		Graduate Students		Under-Graduates		Other Participants[1]	
	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.
A. Total, U.S. Citizens	8	2	2		6	5	1		2	
B. Total, Permanent Residents	1				1	3				
U.S. Citizens or Permanent Residents[2]:										
American Indian or Alaskan Native										
Asian.....	1		1							
Black, Not of Hispanic Origin.....	2									
Hispanic										
Pacific Islander										
White, Not of Hispanic Origin										
C. Total, Other Non-U.S. Citizens					4	4				
Specify Country										
1. China					2	3				
2. India					2	1				
3.										
D. Total, All participants (A + B + C)	9	2	2		11	12	1		2	
Disabled[3]										

☐ Decline to Provide Information: Check box if you do not wish to provide this information (you are still required to return this page along with Parts I-III).

[1] Category includes, for example, college and precollege teachers, conference and workshop participants.

[2] Use the category that best describes the ethnic/racial status fo all U.S. Citizens and Non-citizens with Permanent Residency. *(If more than one category applies, use the one category that most closely reflects the person's recognition in the community.)*

[3] A person having a physical or mental impairment that substantially limits one or more major life activities; who has a record of such impairment; or who is regarded as having such impairment. *(Disabled individuals also should be counted under the appropriate ethnic/racial group unless they are classified as "Other Non-U.S. Citizens.")*

AMERICAN INDIAN OR ALASKAN NATIVE: A person having origins in any of the original peoples of North America and who maintains cultural identification through tribal affiliation or community recognition.

ASIAN: A person having origins in any of the original peoples of East Asia, Southeast Asia or the Indian subcontinent. This area includes, for example, China, India, Indonesia, Japan, Korea and Vietnam.

BLACK, NOT OF HISPANIC ORIGIN: A person having origins in any of the black racial groups of Africa.

HISPANIC: A person of Mexican, Puerto Rican, Cuban, Central or South American or other Spanish culture or origin, regardless of race.

PACIFIC ISLANDER: A person having origins in any of the original peoples of Hawaii; the U.S. Pacific territories of Guam, American Samoa, and the Northern Marinas; the U.S. Trust Territory of Palau; the islands of Micronesia and Melanesia; or the Philippines.

WHITE, NOT OF HISPANIC ORIGIN: A person having origins in any of the original peoples of Europe, North Africa, or the Middle East.