

GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION
RESEARCH PROJECT INITIATION

B
Partially
Approved
OK

Date: March 3, 1976

Project Title: **Chemisorption and Analysis: Carbon Monoxide on Metals and Alloys**

Project No: **E-19-642**

Principal Investigator **Dr. Helen E. Grenga**

Sponsor: **National Science Foundation**

Agreement Period: From 3/1/76 Until 3/31/78

Dr. Cd
31 Jan 80

*24 month budget period plus 6 months for submission of required reports, etc.
Type Agreement: **Grant No. ENG75-16075**

Amount: **\$44,300 NSF (E-19-642)**
7,753 GIT (E-19-332)
\$52,053 Total

Reports Required:

Annual Letter Technical, Final Report

Sponsor Contact Person (s):

Administrative Matters
thru OCA

Mr. Gaylord L. Ellis
Grants Officer
National Science Foundation
Washington, DC 20550
(202) 632-5965

Assigned to: Chemical Engineering

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GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION
SPONSORED PROJECT TERMINATION

Date: 10/20/80

Project Title: Chemisorption and Analysis: Carbon Monoxide on Metals and Alloys

Project No: E-19-642

Project Director: Dr. Helen E. Grenga

Sponsor: National Science Foundation

Effective Termination Date: 1/31/80

Clearance of Accounting Charges: 1/31/80

Grant/Contract Closeout Actions Remaining:

- Final Invoice and Closing Documents
- Final Fiscal ~~Report~~ Accounting (FCTR)
- Final Report of Inventions
- Govt. Property Inventory & Related Certificate
- Classified Material Certificate
- Other _____

Assigned to: Chemical Engineering (School/~~Laboratory~~)

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NATIONAL SCIENCE FOUNDATION
Washington, D.C. 20550

FINAL PROJECT REPORT
NSF FORM 98A

PLEASE READ INSTRUCTIONS ON REVERSE BEFORE COMPLETING

PART I-PROJECT IDENTIFICATION INFORMATION

1. Institution and Address Georgia Institute of Technology 225 North Avenue Atlanta, Georgia 30332	2. NSF Program Engineering	3. NSF Award Number ENG 75-1 6075
	4. Award Period From 3/1/76 To 1/31/80	5. Cumulative Award Amount \$78,716
6. Project Title		

PART II-SUMMARY OF COMPLETED PROJECT (FOR PUBLIC USE)

The purpose of this research was to study the initial stages of adsorption and catalytic decomposition of carbon monoxide on ruthenium in order to identify a mechanistic relation between chemisorption states on specific crystallographic sites and the catalytic activity of these sites. Field-ion and emission microscopy were used to investigate the carbon monoxide adsorption characteristics on the ruthenium. Single crystal spheres of ruthenium were also treated with carbon monoxide at 550°C to determine the activity of various planes for the decomposition reaction; electron microscopy and diffraction were used to analyze extraction replicas of the bulk specimens.

The results of these studies have been published in the literature and, briefly, include the following:

1. Several crystallographic regions on ruthenium, compared to only one previous found on nickel, were active for the decomposition of carbon monoxide.
2. These active regions were composed of surface steps surrounding the three low-index poles, <0001>, <1010>, and <1011>.
3. Two major chemisorption states, α and β , were found on these low index regions.
4. Only one major chemisorption state, β , was found on the inactive or high index regions.

PART III-TECHNICAL INFORMATION (FOR PROGRAM MANAGEMENT USES)

1. IIFM (Check appropriate blocks)	NONE	ATTACHED	PREVIOUSLY FURNISHED	TO BE FURNISHED SEPARATELY TO PROGRAM	
				Check (✓)	Approx. Date
a. Abstracts of Theses		X			
b. Publication Citations		X			
c. Data on Scientific Collaborators		X			
d. Information on Inventions	X				
e. Technical Description of Project and Results		X			
f. Other (specify)					

2. Principal Investigator/Project Director Name (Typed) Helen E. Grenga	3. Principal Investigator/Project Director Signature 	4. Date 8/12/80
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PART III ATTACHMENTS

FINAL TECHNICAL REPORT

INSTITUTION: Georgia Institute of Technology

PRINCIPAL INVESTIGATOR: Helen E. Grenga

NSF Grant Number: ENG 75-16075 A02

GRANT TITLE: Chemisorption and Catalysis: Carbon Monoxide
on Ruthenium

STARTING DATE: 3/1/76

COMPLETION DATE: 1/31/80

PART III

TECHNICAL DESCRIPTION

The purpose of this research was to study the initial stages of adsorption and catalytic decomposition of carbon monoxide on ruthenium in order to identify a mechanistic relation between chemisorption states on specific crystallographic sites and the catalytic activity of these sites. Field-ion and emission microscopy were used to investigate the carbon monoxide adsorption characteristics on the ruthenium. Single crystal spheres of ruthenium were also treated with carbon monoxide at 550°C to determine the activity of various planes for the decomposition reaction; electron microscopy and diffraction were used to analyze extraction replicas of the bulk specimens.

The results of these studies have been published in the literature and, briefly, include the following:

1. Several crystallographic regions on ruthenium, compared to only one previously found on nickel, were active for the decomposition of carbon monoxide.
2. These active regions were composed of surface steps surrounding the three low-index poles, $\langle 0001 \rangle$, $\langle 10\bar{1}0 \rangle$, and $\langle 10\bar{1}1 \rangle$.
3. Two major chemisorption states, α and β , were found on these low index regions.
4. Only one major chemisorption state, β , was found on the inactive or high index regions.

B. PUBLICATIONS:

1. "Thermal Faceting Studies of Tungsten," R. Kumar and H. E. Grenga, *Surface Science* 59, 283 (1976).
2. "Thermal Faceting Studies of Iron," R. Kumar and H. E. Grenga, *Surface Science* 61, 283 (1976).
3. "Catalytic Decomposition of Carbon Monoxide on Single Crystalline Ruthenium," K. Singh and H. E. Grenga, *Journal of Catalysis* 47, 328 (1977).

C. THESES:

K. J. Singh, "Catalytic Decomposition of Carbon Monoxide on Single Crystalline Ruthenium," April 1976. Summary attached.

D. Graduate Students:

1976 - Kamal Jeet Singh
1976-78 - Frances N. Smith
1978-79 - M. Saad
John Mullins

CATALYTIC DECOMPOSITION OF CARBON MONOXIDE
ON SINGLE CRYSTALLINE RUTHENIUM

A THESIS

Presented to

The Faculty of the Division of Graduate Studies

by

Kamal Jeet Singh

In Partial Fulfillment
of the Requirements for the Degree
Master of Science in Metallurgy

Georgia Institute of Technology

April, 1976

SUMMARY

The purpose of this research was to study the interaction of carbon monoxide with single crystalline ruthenium. It was anticipated and confirmed by these experiments that ruthenium catalyses the decomposition of carbon monoxide in the temperature range of 500 to 550°C. An important part of this research was to determine any crystallographic specificity for the decomposition reaction and to correlate these results, if possible, with those on nickel in order to identify active sites for the decomposition.

In many heterogeneous catalytic reactions it is known that the catalytic activity varies with crystal orientation of the catalyst and that relatively few sites on the catalyst surface participate in the reaction. For the catalytic decomposition of carbon monoxide on nickel, it has been shown that these sites are certain steps on one of the low index regions. Carbon monoxide also decomposes on iron, but the formation of carbides prior to that of graphite hinders the identification of active surface sites for the initial decomposition.

A ruthenium single crystal, cut to a spherical shape, was used in this research in order to expose all possible crystal orientations to the carbon monoxide environment. After electropolishing to produce a smooth, strain-free surface, the specimen was annealed in hydrogen, outgassed in vacuum and then treated with carbon monoxide at 500 to 550°C for times varying from 1 to 96 hours.

The effect of crystal orientation on the reaction was apparent

from the resulting pattern of deposition on the ruthenium crystal. The specimen was examined by several techniques, the most successful of which were optical microscopy and reflection high energy electron diffraction (RHEED). RHEED results revealed only graphite on the ruthenium surface; the graphite morphology was then studied with optical microscopy.

Optical microscopy revealed graphite streamers centered about $\langle 0001 \rangle$, $\langle 10\bar{1}0 \rangle$, and $\langle 10\bar{1}1 \rangle$ poles. The deposition began on these low index regions and spread outwards from them. These results are comparable to those on nickel and can also be explained by decomposition of carbon monoxide at steps on these low index regions. A significant difference for ruthenium, however, is the high activity for decomposition on three low index regions, compared to only one for nickel.