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WISCONSIN UNIV-MILWAUKEE DEPT OF PHYSICS
ELECTROMIGRATION AND THERMOMIGRATION IN METALS. (U)
FEB 80 R S SORBELLO

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electromigration electrotransport thermomigration thermotransport electron transport	local field driving forces microscopic field impurity scattering electron-wind force	electron-drag force electrostatic screening Boltzmann equation Liouville equation linear response theory
20. ABSTRACT (Continue on reverse side if necessary and identify by block number)		
The object of this research was to investigate theoretically the driving force for electromigration and thermomigration in metals. The driving force for electromigration was shown to be equal to the local electric field accompanying electron transport. The force was determined from the linear response expression of Kumar and Sorbello using both the Green's function formalism and the Kohn-Luttinger formalism. Corrections to previous force expressions were derived.		

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19. Key Words - continued

grain boundaries	heat of transport
residual resistivity	effective valence
electron relaxation time	phonon scattering
electron mean-free-path	electron-phonon interaction
electrical conductivity	electron-impurity interaction
electron charge density	screening breakdown
Matthiessen's rule	Green's function
Fermi surface	electron self-energy
phase shifts	vertex corrections
de Haas-van Alphen effect	Feynman-Hellmann theorem
dilute alloys	pseudopotentials
liquid metals	lattice distortion
electron structure	fast diffusion
dielectric response	Häffner effect
phase shifts	isotope effect
distorted-wave Born approximation	oscillator strengths
memory function	inversion layer
force-force correlation function	two-dimensional electron gas
ultrasonic attenuation	MOSFET devices
Dingle temperature	activated complex
diffusion	

20. Abstract - continued

The effects of atomic configuration on electromigration was investigated within a pseudoatom picture. Application was made to lattice distortion, fast-diffusers, grain boundaries and isotope effects. Calculations were made of the driving force in liquid-metal alloys and were found to be in agreement with experiment. The Kohn-Luttinger formalism was applied to electromigration in an inversion layer.

The electron-impurity scattering responsible for electromigration was examined. Phase shifts were calculated and related to alloying properties. Agreement with experiment was obtained. The validity of force-force correlation functions in electron transport was investigated. We also considered scattering and screening effects in ultrasonic attenuation.

The driving force for thermomigration was examined. A linear-response expression was derived for the electronic component of the driving force. We calculated this force within Green's function theory.

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RESEARCH OBJECTIVES

The object of this research was to investigate theoretically the driving force for electromigration and thermomigration in metals.

The driving force for electromigration was explicitly shown to be equal to the local electric field accompanying electron transport. The local field was evaluated using a density-matrix formulation and using the Green's function diagrammatic technique. Corrections to previous force expressions were shown to arise from scattering interferences, vertex corrections, and a local polarization effect contained in the off-energy-shell T-matrix. These contributions have been shown to be considerably smaller than the electron-wind contribution in simple metals when the mean-free-path is substantially larger than the electron wavelength at the Fermi energy. Bound states and virtual-bound states were included in the analysis for the first time in any published work. As a virtual-bound state is lowered in the conduction band its contribution to the force continuously approaches that of a true bound state. This would effectively modify the observed electrostatic bare-valence of some impurities, e.g., hydrogen, in metals.

Since the electron wind force is dominant in simple metals and can be most easily calculated using pseudopotential theory, we performed further calculations based on our earlier work. We considered the most realistic atomic configurations to date, incorporating lattice distortion and other structural arrangements never before considered. Lattice distortion effects typically can give 10%-30% corrections to the force. Calculations for the atomic configuration of a fast-diffuser complex show that the structural effects are appreciable and afford a possible explanation of observed anomalous behavior in these systems. Within the pseudopotential picture for nearly-free-electron metals, the structural effects associated with a grain

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boundary have little influence on the driving force for electromigration. Finally, our calculations show how configurational effects may account for the observed isotope effects in liquid metals (Häffner effect) and for an isotope-dependent force in hydrogen electromigration.

Electron-impurity scattering potentials, which would be of use in electromigration calculations, were investigated in terms of the effects they cause in electronic structure. Phase shift parameterization schemes were used and applied to studying the effect of alloying on electronic structure. Effects of lattice distortion were considered. Agreement between theory and experiment was obtained.

Electron transport was investigated within the framework of the Boltzmann equation and within linear response theory. The validity of "memory function" and force-force correlation function techniques was examined. The role of electron-impurity scattering and electron screening effects in ultrasonic attenuation was also considered.

We critically examined the driving force for thermomigration. The phonon-scattering effects require a non-adiabatic analysis. The electron-scattering effects were described by a linear-response expression similar in structure to that used for electromigration. We calculated the force using Green's function theory and obtained results similar to those obtained previously using semi-classical theory.

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PUBLICATIONS

1. Apparent Screening Breakdown Mechanism in Ultrasonic Attenuation, R.S. Sorbello, Journal of Low Temperature Physics 77, 141 (1976).
2. Effect of Alloying on the Fermi Surface, R.S. Sorbello, Physical Review B 15, 3045 (1977).
3. Local Fields in Electron Transport: Application to Electromigration, R.S. Sorbello and B. Dasgupta, Physical Review B 16, 5193 (1977).
4. Basic Concepts of Electro- and Thermomigration; Driving Forces, R.S. Sorbello, Electro- and Thermo-transport in Metals and Alloys, edited by R.E. Hummel and H.B. Huntington (The Metallurgical Society of AIME, New York, 1977), Chapter 1.
5. Electromigration in Liquid Metal Alloys, R.S. Sorbello, Physica Status Solidi (b) 86, 671 (1978).
6. Effect of Impurities on Electronic Structure, R.S. Sorbello, Journal of Nuclear Materials 69, 652 (1978).
7. Microscopic Fields and Currents in d.c. Electrical Conductivity, R.S. Sorbello, Electrical Transport and Optical Properties of Inhomogeneous Media, edited by J.C. Garland and D.B. Tanner (American Institute of Physics, New York, 1978), p. 355.
8. Strong Coupling Theory for the Driving Force in Electromigration, P.R. Rimbey and R.S. Sorbello, Physical Review B, accepted for publication.
9. Force on an Atom in an Electrostatic Field: Feynman-Hellmann Theorem and Oscillator Strengths, R.S. Sorbello and B.B. Dasgupta, Physical Review B, accepted for publication.
10. Electromigration in a Quasi-Two-Dimensional Electron Gas: Theory of the Driving Force, B.B. Dasgupta and R.S. Sorbello, submitted to Physical Review B.
11. Boltzmann Equation and Force-Force Correlation Function for Electrical Conductivity, R.S. Sorbello, submitted to Physical Review B.
12. Effect of Lattice Distortion on Electron-Impurity Scattering: Phase Shifts in the Distorted-Wave Born Approximation, R.S. Sorbello, submitted to Physica Status Solidi.
13. Atomic Configuration Effects in Electromigration, R.S. Sorbello, submitted to Journal of Physics and Chemistry of Solids.
14. Linear Response Theory of Thermomigration in an Electron Gas, P.R. Rimbey and R.S. Sorbello, submitted to Physical Review.

TECHNICAL PERSONNEL

In addition to the principal investigator the following technical personnel have worked on this grant.

Dr. Basab B. Dasgupta

(Postdoctoral Research Associate) -
Theoretician. Worked on Liouville-
equation approach to fields and forces
in electromigration, dielectric response
of electron gas, and electromigration
in a quasi-two-dimensional electron gas.

Dr. Peter R. Rimbey

(Postdoctoral Research Associate) -
Theoretician. Worked on Green's
function theory of electromigration
and thermomigration, with emphasis on
many-body aspects of strong-coupling
theory.

COUPLING

1. The Metallurgical Society of ADME, Fall Meeting 1976

- a. Richard S. Sorbello
- b. Conference (20-23 September 1976, Niagara Falls, New York).
- c. Presented invited paper "Basic Concepts in Electro- and Thermo-migration: Driving Forces."

Also had discussions with R.E. Hummel (University of Florida), P.S. Ho (IBM), H.B. Huntington (RPI), T. Hehenkamp (University of Göttingen), D. Rigney (Ohio State University) and D. Peterson (Ames Laboratory).

2. International Conference on Properties of Atomic Defects in Metals

- a. Richard S. Sorbello
- b. Conference (18-22 October 1976, Argonne National Laboratories, Argonne, Illinois).
- c. Present paper "Effect of Impurities on Electronic Structure."

Also had discussions with C.P. Flynn (University of Illinois), A.M. Stoneham (AERE, Harwell), P.S. Ho (IBM), and R. Benedek (Argonne).

3. APS March Meeting 1977

- a. Richard S. Sorbello
- b. Conference (21-24 March 1976, San Diego).
- c. Presented paper "Local Fields in Electron Transport."

Also had discussions with R. Landauer (IBM), H.B. Huntington (RPI), W.L. Schaich (Indiana University), L.J. Sham (University of California, San Diego), and P. Kumar (USC).

4. APS Topical Conference on Electron Transport and Optical Properties of Inhomogeneous Media

- a. Richard S. Sorbello
- b. Conference (7-9 September 1977, Columbus, Ohio).
- c. Presented paper "Microscopic Fields and Currents in d.c. Electrical Conductivity."

Also had discussions with D. Stroud (Ohio State University), R. Landauer (IBM), A.B. Pippard (Cambridge University), and P.L. Taylor (Case Western Reserve).

5. Midwest Solid State Theory Conference

- a. Richard S. Sorbello
- b. Conference (21-22 October 1977, Argonne National Laboratories, Argonne, Illinois).
- c. Attended sessions and had discussions on electromigration and electron-impurity interaction with W.L. Schaich (Indiana University), P. Vashista (Argonne) and R. Benedek (Argonne).

6. Iowa State University Materials Science Colloquium

- a. Richard S. Sorbello
- b. Colloquium (4 November 1977, Ames, Iowa).
- c. Present review paper to Materials Science Department of Ames Laboratory. Had discussions on electromigration with electromigration experimental group including D.T. Peterson, O.N. Carlson, J.D. Verhoeven and F.A. Schmidt.

7. APS March Meeting 1978

- a. Richard S. Sorbello
- b. Conference (21-24 March 1978, Washington).
- c. Attended sessions and discussed theory of electromigration and electron transport with R. Landauer (IBM), H.B. Huntington (RPI), W.L. Schaich (Indiana University), P. Kumar (U.S.C.), F.M. Mueller (University of Niemegeen), and W.E. Lawrence (Dartmouth).

8. Midwest Solid State Physics Conference

- a. Richard S. Sorbello
- b. Conference (6-7 October 1978, Argonne National Laboratories, Argonne, Illinois).
- c. Attended sessions and discussed electromigration, lattice distortion, and electron transport with R. Benedek (Argonne), G. Mahan (Indiana University) and N.L. Peterson (Argonne).

9. APS March Meeting 1979

- a. Richard S. Sorbello
- b. Conference (21-24 March 1979, Chicago).
- c. Presented paper "Strong Coupling Theory of the Driving Force for Electromigration." Attended sessions and discussed theory of electromigration and electron transport with H.B. Huntington (RPI), W.L. Schaich, G. Mahan and J. Swihart (Indiana University). Discussed experimental possibilities of hydrogen electromigration in palladium with R. Griessen (Vrije Universiteit, Amsterdam).

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