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.
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
- pseudopotentials
- dilute alloys
- lattice distortion
- liquid metals
- fast diffusion
electron structure
- H"affner effect
dielectric response
- isotope effect
- phase shifts
- 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.
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...
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 (Hoffner 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.


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 AIME, Fall Meeting 1976
   a. Richard S. Sorbello
   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
      Gottingen), 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
   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 Califor-
      nia, 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
   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
   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
   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 Niemegen), and W.E. Lawrence (Dartmouth).

8. Midwest Solid State Physics Conference
   a. Richard S. Sorbello
   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
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