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Work by Prof. Joannopoulos and his collaborators is summarized here

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14 June 1994

Dr. George Yoder, Code 1131
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Materials Division
800 North Quincy Street
Arlington, VA 22217

Dear George:

This letter is meant to be a progress report for the period March 1, 1993 to February 28, 1994 of our grant with ONR # N00014-92-J-1752. I am also enclosing a PPPH report for your records.

We continue to make excellent progress towards our goal to theoretically model accurately and understand the properties of interfaces between grains of particles in general and Matrix/second-phase particles in particular. Our accomplishments have been along four directions. Briefly, they are the following:

First, the development of a new theoretical method for performing *all-electron* calculations. The method allows one to by-pass the pseudopotential approximation, yet still retain the flexibility and power of plane-wave expansions. The foundation and success of our method lies in changing the curvature of space in regions of very high electron density. This adaptive Reimannian metric picks the best variational grid for expanding the wavefunctions. Indeed, the new technique provides the same degree of convergence as conventional methods using *twenty times* more basis functions.

Second, the extension and generalization of the chemical concept of electron *softness* to investigate the effects of impurity segregation at grain boundaries. We have successfully demonstrated that one can define a *local softness* for polyatomic systems,

which, when combined with the traditional *softness* characteristics of atoms and molecules, can be used to predict the segregation properties of atoms at grain boundaries.

Third, the development of the first ab-initio theory of dislocation interactions. A variety of interesting results emerge including an ab-initio value for the dislocation core energy; the demonstration that dislocation interactions can approach the classical limit within a few tens of Angstoms; and the discovery of a pathway for the spontaneous mutual annihilation of a dislocation-dipole of the type that occurs when a Frank-Read source emits a dislocation loop.

Finally, an ab-initio calculation of atomic image Scanning Tunneling Microscopy (STM) signatures for Cu, Si and O atoms. Such signatures are crucial in the interpretation of future cross-sectional STM images of Cu/SiO_2 particle interfaces. An example of our theoretical STM images for a perfect $Cu\text{-}SiO_2$ interface is shown in Fig. 1. The region on the left is the Cu matrix. The small bright spots are the Cu atoms. The region on the right is a SiO_2 (α-cristobalite) particle. The large bright clouds are oxygen atoms. The silicon atoms appear only as dark shadows.

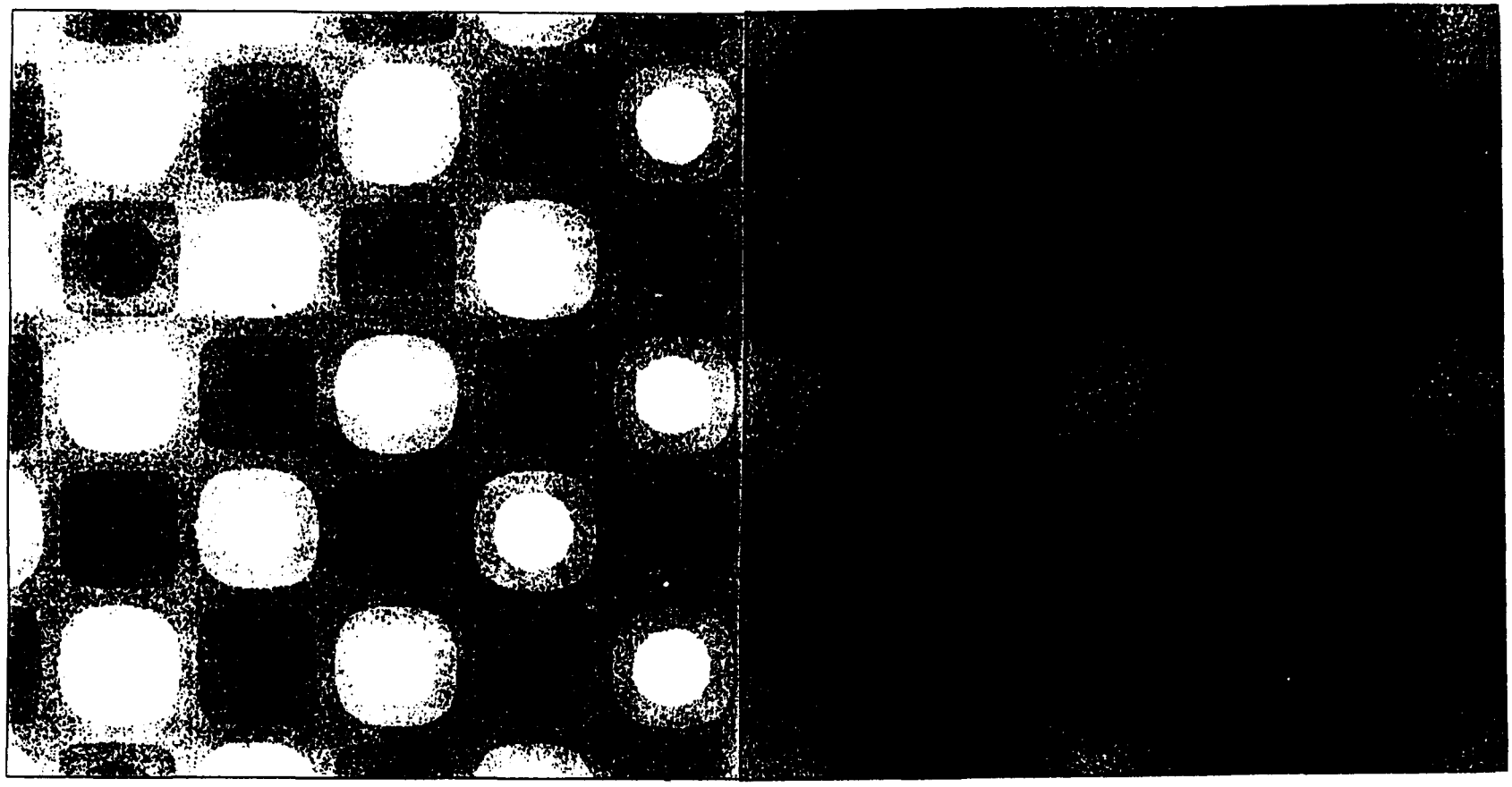
We continue to stay in close contact with Prof. Warren Garrison and his group at Carnegie-Mellon and have piqued his interest in performing crossectional STM studies of his samples as the ultimate way to obtain structural information.

I hope this is sufficient. If you need any additional information please do not hesitate to ask.

Sincerely,

John D. Joannopoulos
Professor of Physics

JDJ:ia



Cu SiO_2

Fig. 1.

OUT vs. (row, col)

OFFICE OF NAVAL RESEARCH
PUBLICATIONS/PATENTS/PRESENTATIONS/HONORS REPORT
for
1 March 93 through 28 Feb. 94

R&T Number: **met0036---01**

Contract/Grant Number **N00014-92-J-1752**
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Principal Investigator: **J.D. Joannopoulos**

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a. Number of Papers Submitted to Refereed Journals but not yet published: **One**

T. Arias, J. Joannopoulos, "Ab-initio Theory of Dislocation Interactions", submitted to Phys. Rev. Letters 1994.

b. Number of Papers Published in Refereed Journals: **3**

K. Cho, T.Arias, J. Joannopoulos, P. Lam, "Wavelets in Electronic Structure Calculations", Phys. Rev. Lett. **71**, 1808 (1993).

A. Devenyi, K. Cho, T.Arias, J. Joannopoulos, "Adaptive Riemannian Metric for all-electron Calculations", Phys. Rev. B.

A. Dal Pino, M. Galvan, T. Arias, J. Joannopoulos, "Chemical Softness and Impurity Segregation at Grain Boundaries", J. Chemi. Phys. **98**, 1606 (1993).

c. Number of Books or Chapters Submitted but yot yet Published: **None**

d. Number of Books or Chapters published: **None**

e. Number of Printed Technical Reports & Non-Refereed Papers:**None**

f. Number of Patents filed: **None**

g. Number of Patents Granted: **None**

h. Number of Invited Presentations at Workshops or Prof. Society Meetings: **None**

i. Number of Presentations at Workshops or Prof. Society Meetings: **None**

j. Honors/Awards/Prizes for Contracts/Grant Employees: **None**

k. Total Number of Graduate Students and Post-Docs Supported at least 25% this year on this contract grant:

Grad Students **1** and Post Docs **1**
Grad Student Female **0**
Grad Student Minority **0**
Grad Stud. Asian e/n **0**
Post-Doc Female **0**
Post-Doc Minority **0**
Post-Doc Asian e/n **0**

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ATTACHMENT NUMBER 2

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Frequency: Annual

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