PHASE TRANSFORMATIONS AND NONEQUILIBRIUM INTERFACES IN ALLOYS.

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F4620-76-C-0103

UNCLASSIFIED AFOSR-TR-80-0177

CARNEGIE-MELLON UNIV
PITTSBURGH PA
Final Technical Report to AFOSR

Agreement number: F44620-76-C-0103

Principal Investigators: J. S. Langer and R. F. Sekerka
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Title: Phase Transformations and Nonequilibrium Interfaces in Alloys

Grant Period: June 15, 1976 through September 30, 1979

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I. Research Accomplishments

The following is a summary list of major research accomplishments during the period of this award. More detailed descriptions may be found in annual technical reports, renewal proposals, and in the publications listed in Section III.

A. Development of a new theory of dendritic solidification: Our new stability theory of dendritic crystal growth appears to be an important advance in the science of solidification. Major accomplishments include:

1) A quantitative theory of the dynamics of sidebranching deformations.
2) Development of a marginal-stability hypothesis which leads to a first-principles prediction of dendritic growth rates.
3) Application of this theory to the study of dendritic growth in dilute solutions.
4) Preparation of a review article on interfacial instabilities and crystal growth to appear in Reviews of Modern Physics.

Relevant publications are numbered 1-7, 9, 13 in Section II.

B. Studies in the theory of directional solidification: This project has focused primarily on the nonlinear theory of cellular solidification fronts. We have succeeded in demonstrating the existence of fully stable cellular structures in one model, and have also explored the behavior of this model in the extreme nonlinear regime. This work recently has led to new results in the theory of eutectic solidification.

Portions of this research are reported in Section V of publication no. 9. More detailed reports will be prepared shortly.

C. Numerical solutions of free-boundary problems: This work has been carried out in collaboration with Professor George Fix of the CMU Mathematics Department and has been supported primarily by CMU's Center for the Joining of Materials. However, the AFOSR contract made substantial contributions to this project during 1978-79. The goal of this project is the development of direct numerical methods for computing the motion of nonequilibrium liquid-solid interfaces under conditions when these interfaces may become morphologically unstable, as in dendritic growth. As a byproduct of this investigation, an AFOSR-supported student has developed and tested a computer program which models welding processes.
The major results of these calculations for the case of an unstable system are reported in publications numbered 11 and 12.

D. Kinetics of phase separation: Our program in precipitation kinetics has focused on both unstable "spinodal" systems and metastable nucleation problems. For solid alloy systems, we have developed a computational method based on the Langer-Baron-Miller (LBM) theory for predicting small-angle X-ray scattering intensities as measured during heat treatments involving experimentally realistic sequences of temperature variations. We also have incorporated hydrodynamic effects into the LBM theory in order to investigate phase separation in binary fluid mixtures. Most recently, we have developed a combined nucleation-growth theory which seems to account quite well for previously unexplained experimental results in near-critical fluid systems.

Relevant publications are nos. 8 and 10.
II. Publications

III. Interactions

The following is a list of invited talks, presented at scientific conferences or at other laboratories, in which research performed under this contract was described.

Lectures presented by J. S. Langer on kinetics of phase separation:
University of Toronto, Physics Colloquium, March 10, 1977.
Materials Science Colloquium, University of California, Los Angeles, January 1978.
Research Institute for Fundamental Physics, Kyoto, July 17, 1978.
University of Hannover, W. Germany, May 21, 1979.
Université Libre, Brussels, May 23, 1979.
Köln University, W. Germany, May 25, 1979.
Aspen Center for Physics, August 1979.
Mid-West Solid-State Physics Conference, Columbus, Ohio, Oct. 9, 1979.
Oak Ridge National Laboratory, November 7, 1979.

Lectures presented by J. S. Langer on solidification theory:
Gordon Conference, July 19-23, 1976
University of Toronto Metallurgy Colloquium, March 8, 1977.
Moscow Seminar on Collective Phenomena, April 18, 1977.
Harvard University, Theoretical Physics Seminar, May 12, 1977.
IBM Research Laboratory, May 17, 1977.
Cornell University, November 17, 1977.
Stanford University, January 5, 1978.
Ames Laboratory, Iowa State University, March 31, 1978.
Chicago Area Solid-State Colloquium April 12, 1978.
Lectures presented by J. S. Langer on solidification theory (continued):
Physiocochemical Hydrodynamics Conference, Washington, D.C.,
International Conference on Collective Phenomena, Moscow, USSR,
December 27, 1978
Symposium of the Division of Condensed Matter Physics, American
Bell Telephone Laboratories, May 1, 1979.

Lectures presented by R. F. Sekerka on solidification theory and nonequilibrium interfaces:
Darken Conference, U.S. Steel Corporation, Monroeville Pa.,
August 1976.
University of Illinois, Urbana, March 1977.
IBM Laboratories, Yorktown Heights, June 1977.
Michigan Technological University, Houghton, May 1978.
American Assoc. of Crystal Growth, Gaithersburg Md., July 1978.
Third European Symposium on Materials Science in Space,
Grenoble, April 1979.
AIMME Meeting, Milwaukee, September 1979.
IV. Personnel

Principal Investigator: J. S. Langer
Co-Principal Investigator: R. F. Sekerka

Postdoctoral Research Associates:

H. Müller-Krumbhaar (1976-77)
A Schwartz (1978-79)
J. Smith (partial support, 1978-79)

Research Assistants:

K. Kasturi (Thesis student, quit for personal reasons, 1976-78.)
P. Popper (Pre-qualifying student 1977.)
R. Mathur (Thesis student, should complete Ph.D in 1980-81.)
V. Datye (Thesis student, should complete Ph.D in 1981.)
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This report describes progress in research on phase transformations and nonequilibrium interfaces achieved during the period June 15, 1976 to September 30, 1979. Major accomplishments include the development of a theory of dendritic crystal growth and performance of calculations pertaining to phase separation in alloys and fluid mixtures.