AD-A119 880 CALIFORNIA UNIV IRVINE F/G 7/4
THE EFFECTS OF SURFACE ROUGHNESS ON THE PROPERTIES OF SOLIDS.(U)
SEP 82 A A MARADUDIN DAAG29-78-G-0108
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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER 15902.5-PH	2. GOVT ACCESSION NO. AD-A119 880	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) The Effects of Surface Roughness on the Properties of Solids		5. TYPE OF REPORT & PERIOD COVERED Final: 1 Jul 78 - 30 Jun 82
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) A. A. Maradudin		8. CONTRACT OR GRANT NUMBER(s) DAAG29 78 G 0108
9. PERFORMING ORGANIZATION NAME AND ADDRESS University of California Irvine, CA 92717		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS U. S. Army Research Office Post Office Box 12211 Research Triangle Park, NC 27709		12. REPORT DATE Sep 82
		13. NUMBER OF PAGES 4
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

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OCT 0 5 1982
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17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

NA

18. SUPPLEMENTARY NOTES

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

surface roughness
image potential
plasmons
Van der Waals forces
wave propagation
light scattering
polaritons
Rayleigh waves

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Published results of work that dealt with various effects of surface roughness on the physical properties of solids are discussed.

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Final Technical Report of Work

Accomplished under Research Agreement No. DAAG29-78-G-0108

During the lifetime of this Research Agreement eight papers were written that dealt with various effects of surface roughness on the physical properties of solids. One more was presented as a contributed talk at a meeting of the American Physical Society. These are listed on an attached sheet.

There are several results of this work that seem worthy of comment. At the methodological level we have developed the so-called "smoothing method" into a useful tool for the study of surface roughness problems, which yields results previously obtained by diagrammatic perturbation theory more simply by algebraic (projection operator) methods. (See, for example, Refs. 1, 6, 7, and 8.)

Our results concerning the effects of surface roughness on the image potential (Ref. 1) have been used by Hipolito and Farias (Surface Science 113, 228 (1982)) in their investigation of the effects of the roughness of the semiconductor/oxide interface on the electronic energy levels of electrons in an inversion layer. They have also been used by Metiu and his colleagues (Chem. Phys. Lett. 85, 404 (1982)) in a study of the fluorescence lifetime of a molecule adsorbed to a rough metal surface. Finally, Marvin and Toigo (Phys. Rev. A25, 782 (1982)) have made use of some of the results of this work in determining the van der Waals interaction between a point charge and a metal surface. Consequently, this one paper in a short time period has had an impact on three rather different types of problems in solid state theory.

The theory of the scattering of a scalar plane wave from a randomly corrugated hard wall presented in Ref. 3 is based on an iterative method for the solution of this problem that has both computational and conceptual advantages over earlier treatments (see, for example, Opt. Comm. 30, 279 (1979)). In particular, it gives a very direct prescription for the separation of the scattered intensity into a specular component and a diffuse component. In addition, it leads in a natural way to the presence of a Debye-Waller like factor that describes the decrease in the specular intensity due to roughness-induced scattering out of the specular beam. This work is now regarded as providing one of the exact solutions to this scattering (M. Nieto-Vesperinas, J. Opt. Soc. Am. 72, 539 (1982)). It has also stimulated two papers in which an improved theory of the Debye-Waller factor for light atom scattering from a low index the surface of a close packed metal has been obtained (N. Garcia, A. A. Maradudin, and V. Celli, Phil. Mag. 45, 287 (1982); N. Garcia and A. A. Maradudin, Surface Science (to appear)). This work is a time-dependent generalization of the work of Ref. 3, in which the random, time-dependent corrugations of a metal surface are due to the bulk and surface phonons of the substrate that give rise to nonvanishing displacements of the surface normal to itself. The theoretical results show that the surface phonons that have been largely ignored in earlier determinations of the Debye-Waller factor in atom-surface scattering in fact play a determining role. The results are in good qualitative and quantitative agreement with experimental results.

Methods worked out and presented in Ref. 6 have been used in two papers (Phys. Rev. B23, 4965 (1981) and Phys. Rev. B24, 595 (1981)) for the determination of the dispersion relations for surface polaritons and plasmons. respectively, propagating across large amplitude dielectric gratings.

In two papers (Ref. 7 and 8) the propagation of Rayleigh surface acoustic waves across a randomly rough, stress-free planar surface of a semi-infinite elastic medium has been studied. In the first of these, Rayleigh's method is used to obtain the dispersion relation for these waves. Their frequency is found to be complex: the imaginary part describes the attenuation of a Rayleigh wave due to roughness-induced scattering of energy out of the incident beam into bulk waves and other Rayleigh waves; the real part is a roughness-induced shift in the frequency itself. In this work it is found that in contrast with the results of earlier work (Ann. Phys. (N.Y.) 100, 262 (1976)) it is the roughness-induced scattering of a Rayleigh wave into bulk waves that is the dominant attenuation mechanism. The reasons for this difference have been explained. The roughness-induced shift in the frequency of a Rayleigh wave has not been studied previously. In the second paper, effective boundary conditions are obtained for the average displacement field in a semi-infinite elastic medium bounded by a randomly rough, stress-free planar surface. These boundary conditions are to be satisfied on the nominally flat surface of this medium, and express the fact that the presence of roughness leads to nonzero stresses acting on this nominal surface. It has been verified that the use of these effective boundary conditions yields the same dispersion relation for Rayleigh waves on a randomly rough surface as does the straightforward application of Rayleigh's method, but the result is obtained more simply. It is expected that the use of these effective boundary conditions will simplify the calculation of several different types of static and dynamic properties of semi-infinite elastic media bounded by a randomly rough, stress-free, planar surface.

In a paper presented so far only at a meeting of the American Physical Society (Ref. 9), a formally exact derivation of the work required to bring a point charge in from infinity up to a randomly rough perfectly conducting surface (the image potential energy) has been presented. This work is based on the extinction theorem form of Green's theorem, and on an exact method for evaluating the averages over the ensemble of realizations of the surface roughness profile that arise. This method makes it possible to study the image potential energy even when the charge is in the selvedge region. The results show that the singularity in the image potential energy as the charge approaches a flat surface is weakened in the presence of the roughness. The methods developed in this paper should make it possible to improve on the theory presented in Ref. 1 by freeing it from the restrictions imposed by the use of the Rayleigh method in that work.

Thus, as a general characterization of the published work done under Research Agreement No. DAAG29-78-G-0108 it can be said that it concentrated on some basic questions of how to deal with surface roughness theoretically, yielded some new physical results, and stimulated work by others.

There are a few pieces of work done with the support of this agreement that have been completed but have not yet been completely written up for publication. These include the work presented in Ref. 9, and a study of plasmons in a dielectric sphere whose surface is randomly rough. Very recently it has been found that the results of this work can be derived more simply and directly by the use of the extinction theorem version of Green's theorem, and the paper describing this work is being rewritten on the basis of this simplification.

The most interesting result of this work is that each plasmon mode of the perfect sphere splits into two modes in the presence of surface roughness. This is reminiscent of the splitting of the surface plasmon dispersion curve for a flat surface into two branches by surface roughness that was discussed in Ref. 2 and by Kretschmann et al. (Phys. Rev. Lett. 42, 1312 (1979)).

There is other work for which the theory has been completed, but the necessary numerical calculations have not yet been finished. One example of this is a study of the image potential energy of a point charge in the vicinity of a perfectly conducting grating surface. A formally exact solution can be obtained in this case that should provide some insights into the analogous problem for a randomly rough, perfectly conducting surface.

These as yet unfinished pieces of work will be completed and submitted for publication, with credit given to Research Agreement No. DAAG29-78-G-0108.

The scientific personnel supported at one time or another by this project have been Dr. A. Eguiluz (Assistant Research Physicist), Ms. J. Shen (Junior Specialist), Dr. David Castiel (Postgraduate Research Physicist), and Mr. Ricardo Gutierrez Lee, Jr. (Research Assistant). Mr. Lee received the Ph.D. degree from the UCI Physics Department for a dissertation written with support from Research Agreement No. DAAG29-78-G-0108.

Papers Written with the Support of
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