ORCA PROPOSAL

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MOLECULAR OPTICS – Reflection and Refraction Calculations on the Atomic Scale

EXECUTIVE SUMMARY

The precise determination of material characteristics – specifically regarding indices of refraction *n* & *k* – affect many applications from EUV (extreme ultraviolet) lithography to high energy space-based satellite telescopes, as well as the more salient optical setups in the ultraviolet and x-ray. Behind these electromagnetic interactions is a setup wherein the placement of individual atoms could affect the outcome of the scattered light. Specifically, the fundamentals of this research deal with the way this energetic light interacts with the material boundaries and composition and the resulting effects that would be seen in the far-field.

BACKGROUND

In the visual regime, the behavior of light is relatively well-understood when it comes to reflection and refraction. Since the wavelength of light in this regime is much larger than the inter-atomic distances, the microscopic or atomic scale does not play a significant role. To a good approximation materials in the optical regime can be treated as bulk, or macroscopic. However, in the EUV when the wavelength of light approaches the inter-atomic distances, the nature of the atomic spacing is important.

Currently, the optical properties of materials are usually computed using bulk properties. At the highest EUV energies this approach becomes questionable. My proposed studies will address the microscopic calculations of the optical properties of thin films in the soft x-ray and EUV regime, where the wavelength is on the order of the inter-atomic distances. I hope to contrast the results of this microscopic research with the results obtained from the 'bulk' method. It is likely that my results will back up the hypothesis that the atomic spacing will affect the optical parameters in the EUV and x-ray. The question is by how much will it affect the outcome?

PLAN & APPROACH

The aim of this project is to obtain qualitative and quantitative results that illustrate the effects the planar boundary and molecular spacing of a material may have on scattering incident photons. A rudimentary program in Maple code has been developed for this purpose and promising preliminary results have been obtained. Unfortunately, this fledgling program still requires development time and effort to achieve its envisioned capacity.

In the program, I will address the amorphous (Gaussian) distribution of the atoms or molecules that would make up the material. The results from this will be compared with the simpler crystalline case, paying careful attention to exactly how the scattering and diffraction patterns may have changed. Next I will incorporate more dimensions into the program. This may involve moving the program into another language in order to decrease computing time. Programming language possibilities include MatLAB, C, and Fortran.

The invoked methods incorporate molecular optics theory with computational work. We will continue to increase the complexity of this program so that it will more closely resemble the actual material.

PROPOSED TIMETABLE

Date	Objective	Specifics
Jan 30	Initiate project	Mentor meeting, theoretical work
Feb 7	Begin programming	Expand 1D amorphous spacing
Feb 14	Program development	Program 'amorphous' in MatLAB
Feb 25	Program development	Expand code in C or C++
March 6	Program, check progress	Half-way meeting, address goals
March 17	Theory evaluation, programming	Explore 2D, 3D amorphous spacing
March 30	Program development	Continue with 2D, 3D
April 5	Continue with program, begin final report	Report to be written in LaTeX to model a publication
April 13	1st draft due	Generate all needful plots for report
April 20	2nd draft due	
June 1	Final report due, wrap up program	Tie up 'loose' researching ends

REPORT CONTENTS

My final report will include a background of this research as well as the results, conclusions, and any research extensions that are realized along the way. Also included will be relevant plots, methods, procedures, and snags.

LIMITATIONS

The nature of this research is slightly open-ended, since my mentor and I are not entirely sure of the outcome, but our main focus will be in the qualitative and quantitative microscopic results. Thus far we have not found anything in the literature that specifically addresses our proposal, and we are anxious to obtain knowledge that we could contribute to the field.

Since our focus is mainly on the effects of variable atomic spacing, we will not be able to research much else outside of this factor.

QUALIFICATIONS

I meet the criteria for eligibility as outlined in the ORCA guidelines. I have also successfully completed two summer REUs (Research Experience for Undergraduates) in astronomy and physics, funded by the NSF (National Science Foundation). In the last year I have presented two posters at conferences, one on celestial mechanics at the January 2002 AAS (American Astronomical Society) meeting in Washington, D.C., and the other on molecular optics at the October 2002 APS (American Physical Society) Four Corners Session in SLC, UT.

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Our studies address microscopic calculations of the optical properties =
of thin
films in the soft x-ray and extreme ultraviolet (EUV) regime when
the wavelength is on order of the inter-atomic distances. =
Investigations
include the effects of surface roughness, as well as one-dimensional =
"amorphous"
atomic spacing, on specular and non-specular reflection.