Molecular Dynamics Simulations of Laser-Induced Surface Acoustic Waves

Cody A. Dennett
Department of Nuclear Science and Engineering, MIT, Cambridge, MA

August 31, 2015

This is all still tied back to the radiation damage problem. The physics behind anisotropic elastic repsonse theory has been known for some time. Similar measurments to the ones that we're working on showing that this is in fact a real effect in single crystal metals has been done for pretty anisotropic materials (see the Cu study from '68). What we're doing that's new is that we can make these measurements with a relatively high degree of precision on materials that are not very anisotropic, Al is one of the closest to tungsten, and we can also get the same measurable changes using molecular dynamics simulations. MD is the key because when looking towards mesoscale problems, you wont be able to plug into analytic formulae to make predictions, you'll need some heterogeneity in the things that you're using to make predictions on measurements that you can't do with the analytical tools at present. If, and since we're seeing this is the case, you can get these same very small scale changes using MD simulations, then they may in fact be the MOST appropriate tool to use in extending this technique for many applications.

1 Introduction

- Motivation
  - The goal of the work is to determine if Molecular Dynamics is an appropriate tool for simulating the linear elastic response of materials to the type of excitation used in transient grating spectroscopy for single crystal metals.
- What we did
  - Measured the Rayleigh wave velocity of single crystal aluminum oriented at {100} and {111} using several different wavelengths of acoustic wave.
  - Measured the anisotropy of Rayleigh wave propagation with respect to relative orientation on the surface of single crystal aluminum and tungsten samples.
  - Simulate in MD the Rayleigh wave response of {100} and {111} oriented aluminum at several length-scales.
  - Simulate in MD the change in Rayleigh wave velocity with relative orientation on several surfaces of aluminum and copper.
  - Make analytical predictions of the variation in surface wave velocity with relative orientation on single crystals using the elastodynamic Green's function formulation ala A. G. Every.
- What we get
  - Excellent scaling between experiments on the single micron wavelength scale and MD simulations on the tens of nm wavelength scale.
  - Agreement between theory, simulation, and experiment on the degree of variation in the Rayleigh wave speed with relative orientation.
- Use
  - The ability to uniquely determine the orientation of unknown, low-index, single crystals using a combination of either MD simulations and experiment or theory and experiment. High-confidence predictions rely on absolute calibration using a sample of known acoustic properties such as single crystal tungsten.
    - Compare to current techniques that are big, slow, and expensive like EBSD, Laue backscatter diffraction and XRD.
  - Clear bound on the uncertainty of experimental Rayleigh wave velocity measurements based on statistics and accounting for relative orientation effects in single crystals.
    - Reference UK method for orientation mapping. Mention that this technique is reliant on textbook values of elastic constants as inputs and is not readily generalizable to cases in which mesoscale defects effect the elastic properties of materials under investigation.
  - Confidence in MD as a tool to simulate this types of responses. Allows for exploration of effects of mesoscale defects on Rayleigh wave propagation which cannot be easily accounted for in theory but are in fact areas of interest in experiment.

2 Methods

- Material Choice
  - Aluminum: Focused efforts of this study on Al since it is a relatively isotropic material. If we are sensitive to the small changes in SAW velocity expected with relative orientation change on the surface in both experiment and simulation then that is a strong indicator of simulation performance.
  - Tungsten: Chosen as an experimental calibration standard, at {100}, since it is the most isotropic simple metal. Expect and see little variation experimentally at different orientations along the surface.
  - Be sure to mention surface preparation for both of the experimental samples.
  - Copper (?): Chosen as additional simulation case since it is a more anisotropic material and shows that potentials for a variety of materials are available and appropriate to make the kinds of predictions we're interested in.
- Experimental Methodology
  - Experiment description including discussion of heterodyne detection for signal amplification. This include a **diagram of the experimental setup**, which may need to be modified after I finish re-aligning the setup.
  - Power, rep rate, spot size, grating spacing, and sample management (rotation stage) parameters detailed.
  - Data processing: Heterodyne phase correcting, non-exponential thermal decay subtraction, derivative taking, periodogram taking, peak finding, and velocity calculations from measured calibration sample from each run.
- Molecular Dynamics Methodology
  - Simulation volume construction including various sizes under investigation.
  - Discussion of potential that is used for the simulations.
  - Excitation method and similarities to experimental excitation.
  - Relative orientation changes and how they're implemented within the framework of corresponding to experiment. **This is where a figure of both the simulation volume and how its oriented would be helpful.**
  - Data recovered (z-tracking) and processing procedure, sensitivity to motion orthogonal to the surface only.
- Theoretical Predictions
  - Based on the methodology presented by Farnell in Physical Acoustics vol. VI.
  - Need to hear back from A. G. Every before I can more accurately write to this point.

3 Results

3.1 Experimental Results

- Al {100}
  - Measurements at 4-5 different grating spacings (2.05, 2.75, 3.7, 4.x, 5.5 um).
  - Measurements over 180° in 10° increments, known symmetry periodicity.
- Al {111}
  - Measurements at 4-5 different grating spacings (2.05, 2.75, 3.7, 4.x, 5.5 um).
  - Measurements over 120° in 10° increments, known symmetry periodicity.
- W {100}
  - Measurements over 180° in 10° increments, known symmetry periodicity. Make these measurements with goal of finding no change and using the statistical error we find as a baseline for the error in our experimental SAW velocity determination.

3.2 Theoretical Predictions

- Al {100}
  - Predicts a xx% variation with a periodicity of 90%.
  - Possibility of PSAWs?
- Al {111}
  - Predicts a xx% variation with a periodicity of 60%.
  - Possibility of PSAWs?
- W {100}
  - Predicts a xx% (small, resolution defining) variation with a periodicity of 90%.

3.3 Molecular Dynamics Results

- Al {100}
  - Scaling, measured at nine different effective SAW wavelengths.
  - Relative orientation, measured at xx wavelength. Data taken along xx directions on each surface which should correspond to the minimum and maximum speeds along that surface.
  - For all of these simulations, discussion of the number of modes you see in the response. You'll see the plate mode since the simulation volume in line with the excitation direction is so thin. It is the next mode up in frequency that corresponds to the SAW that is detected in experiment. See this as the lowest order mode is the same for different orientations of Al.
- Al {111}
  - Scaling, measured at six different effective SAW wavelengths.
  - **One figure with scaling data from both orientations of Al.**
  - Relative orientation, measured at xx wavelength. Data taken along XX directions on each surface which should correspond to the minimum and maximum speeds along the surface.
- Cu {100} (?)

4 Discussion

- Comparison of experiment, theory, and simulation
  - This can be best accomplished in a table which lists the relative change in SAW speed with orientation, the biggest percent variation, from theory, experiment and simulation. Make sure to note the lengthscales used for experiment and simulation.
  - Note that to reasonable agreement everything works out, all of the variations are on the same percent scale, and maybe even work in a plot once we can normalize for actual speeds plotting all these against each other. ← That would be really interesting to see for one case.
- The rest of the discussion points have already sort of been mentioned under "Use" that is in the intro now.
- Unknown crystal orientation
  - We again show the use of this technique to determine unknown single crystal orientations coupled with theoretical predictions of the SAW velocity. However, what we get now is the ability to make the same sorts of predictions using simulations and not theoretical predictions. This is the key, because theoretical predictions rely on elastic parameters as inputs and if you have a material with some manner of defect population that will change the effective elastic parameters, then you can no longer rely on theoretical predictions to allow you to accurately predict orientation. The kicker is that using MD simulations, you can in fact account for the possibility of defect populations and allow yourself to being to identify classes of non-ideal materials.
- MD as an appropriate tool
  - Similarly to the point above, we see that MD simulations used in this way are sensitive enough to show these single percent changes in acoustic properties and effectively return the same information as experiment. This indicates that MD may in fact be THE most appropriate tool to explore the effects of mesoscale defects on the SAW responses of materials.
  - If one is interested, like we are in the field of radiation damage, in studying the effects of single and multiple classes of defects on the elastic properties of materials, then MD seems to be a complimentary tool for the cases in which theory with *a priori* knowledge of elastic constants fails. Especially in the case of the reverse problem, when you are seeking to explore the effects of mesoscale defects on the elastic constants.
  - This maybe should go before "Unknown crystal orientations".
- Bounds on experimental uncertainty
  - Although important, I'm not sure if a detailed discussion of this point fits in with the scope of this work, besides a mention of how we're handling uncertainly and its propagation in the experiment section.
  - It may be best to use this paper as a reference in the future for a beginning on the bounds of what we can detect and since we're not talking specifically about radiation damage effects on the sub-percent scale yet, we may not need to mention anything explicitly.

5 Conclusion