Molecular Dynamics Simulation of Thin Film Conductor Tensile Properties

(Technical Paper)

Informational Apathy: The Impact of the Information Age

(STS Paper)

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On my honor as a University Student, I have neither given nor received unauthorized aid on this assignment as defined by the Honor Guidelines for Thesis-Related Assignments

Introduction

With the advent of the information age, the nature of popularity has changed. Instead of word-of-mouth, popularity is often determined by one of many algorithms. And those algorithms, in turn, make decisions based on individual preference. Popularity has become both personalized and artificial; the STS proposal will explore what this means both for individuals and groups. In particular, the role communications technologies, particularly social media, algorithmically curated news feeds, anonymity and/or pseudo-anonymity, and communications technology play in developing previously insignificant or nonexistent niche communities (echo chambers) will be explored. The thesis will analyze how these niche communities contribute to information disorder and misinformation on the internet and in the information age, and what demarcates a benign community from a malignant one. (Wardle & Derakshan, n.d.) Lastly, the responsibility of companies, individuals and governments regarding these niche communities and their strengthening factors will be discussed, and what each of these parties can do to mitigate the presence and effect of echo chambers in communications technology.

Humans are slow to adapt to new technology; our society must think ahead about how these technologies will affect us, our loved ones, our institutions and relationships. Like many emerging technologies, communications technologies have the potential to control us and the way we behave, and so all of us have a responsibility to understand them, and both regulate ourselves and these technologies so that they remain tools as they mature, so we can make them as beneficial and useful as possible. The development of cloud computing, feed and search algorithms, the internet and other communications-enabling technologies has been founded on the exponential development of increasingly powerful hardware. The technical topic involves basic research in the field of thin-film conductors, and is motivated by a need for increasingly

versatile electronics. Demand for flexible electronics exists in the fields of prosthetics, wearable electronics, biomedical engineering, embedded electronics, lighting and photovoltaics. (*The Flexible Electronics Opportunity*, 2014) Many devices and potential devices have constraints that prevent a rigid semiconductor or fiberglass chip from being embedded in them, or their value is increased without rigid electronics. The research performed in Professor Xu's lab of the Mechanical Engineering Department and will support and improve the consistency of aqueous thin film peeling, one technique for creating flexible electronics.

Technical Topic: Thin Film Conductor Stress-Strain Behaviour in Aqueous and Aqueous-Vacuum Interface Conditions

The technical project will involve molecular dynamics (MD) simulations[1] of tensile tests[2] of different thin-film conductors in submerged aqueous, and aqueous-vacuum interface conditions.[3] The research question being asked is what the molecular mechanism that causes deviation of Young's Modulus in thin films from bulk materials. Two different materials (pure gold and nickel) will be tested in both conditions. These materials were chosen both due to their relevance to thin-film electronics. Each material will be tested at different thicknesses (2nm, 5nm, 10nm, 20nm). It has been demonstrated that Young's modulus in aqueous-vacuum interface conditions does vary with thickness (Kim et al., 2013), however, the mechanism for this variance is unknown. It is hypothesized that size effects due to increased surface area-to-volume ratio change the fracture mechanism, reducing the energy required to neck and fracture the

[1] Molecular Dynamics involves the use of discrete mathematical models that approximate classical physics on a molecular scale to simulate the outcomes of nanoscopic systems on picosecond timescales.

[2] A common procedure in materials science used to determine elastic and plastic moduli, toughness and a few other material properties.

[3] "Completely submerged in water" and "floating on the surface of water," respectively.

material. Additionally, this study may be extended to study nanofilms composed of a graphene-gold bilayer. It has been shown experimentally that such a material has a completely different fracture mode than pure gold or graphene nanofilms, but like the difference in Young's modulus, no mechanism explaining this difference is known.

This research is relevant to the field of flexible electronics, a method of creating flexible electronics explored in the Xu lab is mechanical peeling of thin films in aqueous conditions. Predicting the behaviour of these peeling thin films can be difficult however as their elastic behaviour is different than that of bulk materials. This study seeks to understand the molecular mechanism explaining this difference in behaviour will allow better prediction of thin film behaviour during mechanical peeling manufacturing of flexible electronics, and reduce the trial-and-error involved in designing procedures for thin film peeling.

This research will be conducted largely independenty, with advising from Professor Baoxing Xu, using resources from the Xu Lab, over the course of the academic year. The first semester will be spent getting oriented with relevant tools, such as LAMMPS, moltemplate, VMD and topotools, as well as doing literature research and review on molecular dynamics methods relevant to this simulation; primarily finding pair potentials and relevant parameters and testing them. The first half of experimentation will also be performed towards the end of the first semester, establishing simulation setup, testing gold in submerged conditions and troubleshooting. Winter break and second semester will be spent testing aqueous-vacuum interfaces, nickel, and larger, thicker samples of both materials; if time permits, graphene-gold bilayer simulations will be performed as well. Ideally, this research will result in data that can be published, and lead to a theory describing Young's modulus in thin film conductors.

STS Topic: Algorithmic Popularity; the Filter and the Feed

The STS proposal is an analysis of artificial popularity, particularly algorithmically curated feeds, communication technologies, the echo chambers that they create, and what can be done to mitigate or regulate the more malignant of these echo chambers.

As of this writing, feeds are often the home pages of not only social media websites (Facebook, Twitter, YouTube, Instagram, etc.), but also any content services (the iOS App Store and Forbes, for example). Any website with a backlog of interrelated and interlinked content can benefit from an algorithmically curated, infinite feed. Feeds allow content services to deliver content that is interesting to users on an individual basis, increasing user retention and ad revenue. Little academic research has been completed about the effects of these feeds, most information regarding them is largely opinionated journalistic articles or what little information communication services make public about these algorithms.

This property of feeds results in a phenomenon called filter bubbles, or echo chambers. Echo chambers result when an individual surrounds themselves with information sources and other individuals that reinforce their preexisting beliefs. (Quattrociocchi, 2017) While this is not a new phenomenon, and is fundamentally based in classical psychology's confirmation bias, it is uniquely enhanced by content and communication services. (Nickerson, 1998) Feeds particularly enhance this phenomenon because they allow for individuals to feel validated by a community without needing any direct person-to-person interaction, allowing a community to radicalize around its content as opposed to its interactions, lowering the barrier to radicalization. (Davidson, 2017; Solon, 2017)

Designed to optimize metrics such as view time, meaningful experiences or user enjoyment, feeds largely exclude content irrelevant to the user's interests. In some cases, both

users and content creators can consciously or unconsciously manipulate feeds so that they show largely untruthful or destructive content. (Tien, 2018) Furthermore, the companies that create these algorithms are not infallible and inherently driven by profitability, leading to some manipulations of the algorithm to their own benefit. (Morris, 2019) These factors have combined to increase the spread and reinforcement of conspiracy theories, use of social media in an attempt to manipulate elections, and movements that have real impact and harm, including the antivax movement, "bleach therapy," pro-self-harm movements and various unfounded "health movements," such as the keto diet. (Harison & Zane, 2017; Hussain, Ali, Ahmed, & Hussain, n.d.; Morello, n.d.; Sharrock, 2013; "Should you try the keto diet?" n.d.). Whereas feeds are governed by controllable algorithms, echo chambers form naturally, and naturally retain members because of their exclusionary nature. This results in radical closed-mindedness, and in the cases of some more influential echo chambers, generates a wicked problem, as individuals isolate themselves from information that could correct their thinking. (Kruglanski, 2004) Some arguments have been made for using Feeds to mitigate filter bubbles by displaying validity information (Pennycook & Rand, 2019), however this would demand change by the social media networks themselves.

The relationships between algorithmically curated feeds and communications technologies, the companies that build them, the niche communities they create, the individuals that use them, and governments that are beginning to regulate them, will all be explored. As these are components and shareholders in a literal network, actor-network theory (ANT) will be applied. (Cressman, 2009) While ANT is often criticized for being overly broad and encompassing, it will be restricted to looking at relationships between technologies that directly relate to people, people themselves, and groups composed of people. Social media services are

literal networks composed of people, groups and companies, and so analyses of the networks that built them up is particularly applicable.

This research is relevant as social media services and other communications services develop. While these services become popular due to broad appeal by the companies that create them, the changes that are made to them once they have gained popularity often affect and contort the way popularity works on these platforms. As a result, information shared through these services often becomes biased, even as it reaches individuals. It is important, therefore, to understand these effects, so that the individuals that use these services might understand how to avoid the trappings of echo chambers and other pitfalls of the technology; and also so that these individuals might call for regulation of these technologies from either the companies that run them, or governments that regulate communications technologies. Research for the STS topic has begun in the Fall 2019 semester, and will be completed and culminate in a paper during the Spring 2020 semester.

Research Questions and Methods

Do feeds and communication technologies combine to create a more narrow-minded individual by developing echo chambers and niche communities? Is this the responsibility of the social media company as the curator of algorithms that create these bubbles in the first place? Can this problem be fixed through social or technological means, or must the solution be political?

In particular, exploration of whether or not an algorithm can be designed that is resistant to creating filter bubbles is possible, whether or not individuals can be made aware of and convinced to avoid or leave filter bubbles (research shows this is not promising; attempted debunking often reinforces held beliefs (Lewandowsky, Ecker, Seifert, Schwarz, & Cook, 2012; Quattrociocchi, 2017)); and whether or not this is something worth regulating through policy. This question is most obviously amenable to wicked problem framing. The standing problem of filter bubbles immediately seems "wicked" because individuals within one or more of these bubbles would be conditioned to reject any accusations that the communities they have restricted themselves to are biased and narrow-minded. Even if these accusations made it through said filter bubble in the first place, they would be quickly swept away by the feed, which is inherently temporal.

This question is also strongly aligned with documentary research methods in conjunction with discourse and network analysis. As social media *networks* are inherently platforms on which individuals carry out *discourse,* although an argument could be made that it is more like reciprocal broadcasting than discourse much of the time.

Much of the language on misinformation research has been established in Wardle and Derakshan's 2019 Information Disorder report, which will be used in the discussion of filter

bubbles. Filter bubbles themselves are outlined and explored in Quattrociocchi's papers. Once these basics concepts have been established, the remainder of the proposal will be spent analyzing available information regarding the new feeds algorithms created by social media companies, how they affect individuals, and how they have been, are, or may be regulated, in that order.

Conclusion

The technical deliverable will be quantification of reduction in Young's modulus in correlation with decreasing sample thickness for metallic thin films in aqueous and aqueous-vacuum interface conditions. Visualization of and theorization on the mechanisms that cause this observed reduction are the ultimate goals of this study, with a long-term significance of increasing the predictability in thin-film peeling manufacturing methods for flexible electronics.

The STS deliverable will involve an analysis of filter bubbles and feeds in the context of niche online communities, an exploration of how they can interact to produce narrow-mindedness in users of social media and other online communication platforms. This will end with a discussion of responsibility for these algorithmically driven artificial popularity systems and a discussion of different potential solutions to the filter bubble phenomenon. As communication technology becomes more pervasive, it becomes increasingly necessary to understand how it affects our behaviour, and how we, both as individuals and as a society, can mitigate and regulate the more negative effects, so that we can enjoy the beneficial aspects of communication technologies.

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