A Quantum Field Theoretic Approach to Disordered and Amorphous Solids

The objective is to formulate a fundamental theory of defects in disordered solids using quantum field theory (QFT) methods, with the ultimate goal of understanding amorphous materials.

Motivation: P. W. Anderson said in 1995, "The deepest and most interesting unsolved problem in solid state theory is probably the theory of the nature of glass,[1]" glass being the prototypical highly-disordered amorphous material. Defects describe disordered materials in a more concrete, physical way, and are central objects of study in materials science. They govern the deformation of solids and overall mechanical properties, but also significantly affect electronic, optical, and other functional properties.[2] This alternative approach to disordered systems holds great promise.

Due to their long-range nature and effects, extended defects in particular, including dislocations, grain boundaries, etc., are difficult to model and not well understood theoretically. Common computational methods like density functional theory (DFT) scale poorly with system size, making such defects too costly for simulation.[2] Classical molecular dynamics is based on Newtonian mechanics, so doesn't take into account any quantum effects. While there exist empirical models for the effect of defects on these functional properties, they need many parameters, and none are fully *ab initio*. A radically different approach is needed.

Introduction and Background: The classical theory of dislocations more or less fully explains mechanical properties of materials. However, there remain many open questions on how dislocations and defects in general affect functional properties, that remain so because the classical treatment is insufficient. I propose to describe extended defects in disordered solids as quantum fields that give rise to quasiparticles, enabling a deeper understanding of defect interactions. Motivated by the example of phonons as quasiparticles that quantize the lattice displacement field, we define a new quantum field for dislocations and its associated quanta – the "dislon"[3]. Much as the phonon theory led to great advances in understanding the effect of lattice vibrations on photons and electrons, this new theory will lead to a similar paradigm shift.

Initial Successes–the Dislon: A dislocation is an extended crystal defect. Critical to formalizing them is the Burgers vector **b**, representing the dislocation-induced lattice distortion and associated displacement field **u**. This **u** is the classical field we turn into a quantum field for the first quantization. Conceptually, the constraint imposed by **b** is very important, as the only thing distinguishing a phonon from a dislon, both being just quantized **u** at heart.

Already this theory has been successfully applied to supplant previously incomplete explanations of materials phenomena, such as the effect of dislocations $\frac{g_D/g_{ph}}{\Gamma_D/\theta_D} \propto \left(\frac{1-\nu}{1-2\nu}\right)^2 \frac{k_F^2}{m^* L(\lambda+2\mu)b^2} \frac{\theta_D N(\mu)}{N(\mu) g_{ph}}$ on superconducting critical temperature T_c. The expression above is analytically derived and describes the competition between quantum vs. classical effects.[3] It predicts the direction of T_c change after increasing dislocation density, which affects Poisson's ratio ν and Lamé parameters λ, μ. It is somewhat surprising because the expression combines variables/parameters describing both mechanical and electronic properties, not usually seen together in one formula.

Research Plan: I plan to join the Energy Nano Group, led by Prof. Mingda Li, creator of the dislon theory. His group combines theory and experiment, and I will contribute to the theory side of research. With the dislon as the origin, we can organize our future work along three axes.

Axis 1–Deepening: The dislon theory still has great potential to be applied to many other types of interactions. One example is dislon-induced topological phase transitions, where we turn a topologically trivial material into a topological insulator by tuning its bandgap. I will include electron-dislon interactions into band structure calculations, which avoids the computationally

expensive supercells required for DFT. Another application is dislon-enhanced Anderson localization, the suppression of electron diffusion in disordered systems.[4] Dislons give us a way to explore this effect in crystalline materials, which thus far has been challenging to observe.

There is still much work to be done extending the theory itself. Most promising is the incorporation of gauge symmetry, a classical theory of which already exists for dislons.[5] The goal is to quantize this, analogous to quantum electrodynamics (QED) for electrons. In the same way photons arise naturally from QED as a force carrier, we would expect something similar from a quantum gauge theory of dislons, that can shed light on the nature of plasticity.

Axis 2–Broadening: The quantization procedure outlined for dislons can be readily generalized to account for anisotropy and discrete lattices (current derivation is for continuum limit). The initial success with dislons means this is a promising approach to defects in general. In conjunction to the work **Axis 1** on 1D dislocations, I will generalize the quantization process to 2D grain boundaries and 3D inclusions. An analytical theory allows computation of interfacial transmission coefficients for the Landauer formula from microscopic and no *ad hoc* parameters.

Axis 3–Experimental: There will be a strong experimental component to inform and augment the theory development. Working with our collaborators at Oak Ridge, we will probe phonon-dislon interactions using advanced techniques like inelastic X-ray and neutron scattering, to see if measured thermal transport and relaxation coefficients match those calculated from dislon theory. Additionally, we will use our lab's crystal growth facilities to synthesize materials with controlled dislocation density, to explore dislon-induced topological phase transitions.

Intellectual Merit: With the dislon model, all dislocation effects are incorporated: strain, coulombic, and vibrational. We now have a systematic framework to investigate the effect of defects on functional properties, by including a defect Hamiltonian. This allows us to calculate constants such as deformation potential coefficient *ab initio*, which will lead to a deeper understanding of material properties far beyond any empirical model. We can also now use tools from QFT like Feynman diagrams to study complex electron-phonon-dislon interactions.

One may ask, why should extended defects be quantized to begin with? The intuition is that extended (as opposed to point) defects have spatial extent, captured by the "field" part of QFT, and its resulting internal dynamic structure is described by the "quantum" part. We have shown this idea applies to dislocations, suggesting it applies generally to all extended defects.

Broader Impacts: These theories will have a profound impact on the direction of condensed matter and materials research. Much work now is on trying to find new materials with desired properties. By understanding how defects can induce such properties, we vastly expand the family of known materials exhibiting them, without needing to find completely new materials.

As a radical theory that sits at the intersection of quantum field theory and materials science, two disciplines with relittle crosstalk, there is much educational potential. Through talking with my colleagues in the materials science department, I aim to start bridging the gap between these two communities. I plan to help develop a course introducing QFT to engineers, that I could be a TA for, and eventually down the line, perhaps even write a textbook on this theory.

So far, over 20 years after Anderson's comments, we still only have the empirical model of electrons in glass developed by Mott.[1] By understanding defects, we hope to ultimately have a fundamental theory of amorphous materials, as a limiting case of infinitely many defects.

Works cited: [1] Anderson P W, *Science* **267**, 1615-16 (1995) [2] Mott N F and Davis E A, *Electronic processes in non-crystalline materials* (2012) [3] Li M, *arXiv preprint*, *arXiv:1808.07777* (2018) [4] Anderson P W, *Phys Rev* **109**, 1492-505 (1958) [5] Kadic A and Edelen D G B, *A gauge theory of dislocations and disclinations* (1983)