PhD Thesis Title: Plasmon Phonon Coupled Dynamics of Nanocrystalline Structures

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Abstract:

This thesis is an attempt to understand the characteristics and responses of plasmon phonon coupled dynamics in nanocrystalline structures. An energy based Lagrangian formulation is developed with fundamental field quantities like displacement, charge, electric and magnetic field as variables. Governing differential equations of motion are derived from variational calculus. A new computational framework is implemented to solve for system degrees of freedom, which involve energy and force exchanges between atomic and continuum representation of the system. The developed simulation framework is employed to investigate the phonon and plasmon characteristics for nanocrystalline copper thin films and carbon nanotubes under decoupled scheme. Several fundamental properties are estimated which are found in agreement with experimental and first principle calculations. The simulation framework is applied to analyse the coupling behaviour in a nanocrystalline copper, free standing structurally engineered graphene, pure carbon nanotubes, macromolecular carbon nanotube composite structure, engineered graphene on a silicon substrate and zinc oxide on a zinc substrate. Intense coupled modes are identified using these material models to demonstrate the usefulness of the developed framework and simulation results. The one-dimensional ultrathin copper nanowire has shown the existence of optical phonon modes in copper. Three different plasmon extinction peaks are observed for nanowire. The coupling between the plasmons and optical phonons is reflected in the form of splitting, screening and intensity rise in the phonon density of states. Device configuration with nanowire mounted on a substrate shows a strong excitation of surface plasmon and the phonon oscillations. The charge localization near the defect induces a secondary plasmon excitation. The repetitive electromagnetic irradiation heats up the graphene lattice and achieved a complete screening optical phonons. Uncontrolled heating initiated a lattice failure in graphene with hole defect. A good control on transport of thermal energy is achieved with the help of graphene boundary engineering. The coupled analysis for a single walled carbon nanotube is estimated under controlled temperature at different stages of mechanical elongation. A step wise decay in the plasmon energy is observed with increased in the lattice strain. The local plasmon induced electric fields modulate the phonon intensity and mode switching in strained nanotubes. Macro-molecule involved nanotube binding and the coupled characterstics are analyzed. The combination of zinc oxide nanowire with zinc substrate shows a decrease in the plasmon energy due to the chemical bonding between them. The experimental equivalent growth process is modeled using atomic interaction potentials. The nucleation of zinc oxide from the zinc substrate was confirmed with the bond legth, bond angle and charge computations. The thermodynamic stability of graphene on silicon substrate is investigated through the variation of bond energy and bond density with graphene orientation. A global minimum is found in middle of armchair to zigzag configurations. The silicon-graphene shows two extinction peaks ans strong difference in the plasmon induced coupled phonon mode of vibration. The developed theoretical model and its numerical implementation are useful to get a higher level understanding of dynamical behaviors of various nanoscale devices.