Multiscale flexoelectric modelling

Two-dimensional materials for energy storage and harvesting

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In Short

- Develop simulation models to study the flexoelectric energy generation in novel two-dimensional materials.
- Utilize machine learning techniques to derive the inter-atomic potentials.
- Investigate the flexoelectric effect in nanostructures from two-dimensional materials and their assemblies.
- Accomplish macroscale energy storage and harvester models based on the nanoscale input.

Two-dimensional (2D) materials have been widely studied due to their exceptional properties. The energy generation using electromechanical effects is an emerging area of research in 2D materials, which appreciates harvesting the energy in ultra-small devices and avoiding the use of hazardous battery materials in sensitive applications. In this direction, piezoelectricity, the best-known mechanism for converting mechanical deformation into electrical energy. However, piezoelectricity is limited to materials with noncentrosymmetric crystal structures. The other type of electromechanical coupling, flexoelectricity, attracts significant interest by ignoring material symmetry. The flexoelectric polarization relates to both strain (as in piezoelectricity) and strain gradient. As the dimension of the 2D materials reduces to nanometer scale, it is likely to produce larger strain gradients that drive for flexoelectricity. Authors' recent study [1] reports the generation of electrical voltage (in mV range) using the flexoelectric effect, where the electricity is induced by mechanically crumpling of the graphene sheet. Additionally, we employ machine learning interatomic potentials to derive the flexoelectric proparties of diamane monolayers [2].

The one-dimensional nanostructures (1D), such as nanotubes, wrapped from the 2D materials known to exhibit the piezoelectric properties. Especially for boron-nitride nanotubes (BNNT), the tensile and twisting piezoelectric properties predicted from the atomisitc finite element method combined with molecular mechanics [3]. However, the methodology involved in that study is not applicable to extract the flexoelectric response. The high strain gradients near the carbon and boron-nitride nanocone apex result in generating a high dipole moment (flexoelectric effect) [4] [5]. These studies are limited only to explain the dipole moments and not extracted the voltage or electrical quantities. Further, their applicability is limited in predicting the nanostructure assembly. Worthy to note an experimental realization [6] about harvesting the electrical energy from the tensile or torsional deformation of a carbon nanotube (CNT) yarns.

In this project, we aim to investigate the flexoelectric effect in largely deformed 2D materials and different nanostructures. By knowing the nanoscale flexoeelctric responses, we then build macroscale models for the energy storage and harvesting applications. The designed work packages (WP) briefly discussed in the following.

WP1: Flexoelectricity in 2D materials with large deformations

In order to study the flexoelectric response for 2D materials, we perform molecular dynamics (MD) simulations by utilizing the charge-dipole (CD) model in conjunction with short-range bonded interactions to determine the atomic configuraitons, as well as charges and dipole moments. We employ machine learning techniques to derive the short-range atomic potentials and perform first-principle simulations to find the CD model parameters. According to the CD model, the total electrostatic energy is a sum over charge-to-charge, charge-to-dipole and dipole-to-dipole interactions. The solutions of equilibrium equations from the energy functional result the charge and dipole moment of every atom. This information is utilized to update the atomic configuraiton. In order to ger the large-scale deformations under indentation, we define a load cycle that prescribes atomic displacement for a shorter period of time followed by a longer relaxation time keeping the indenter fixed. During the evolution, the atomic configuraiton, charges, dipole moments, electrical fields, voltage, etc are stored at frequent time intervals. By processing the generated data, we explore the felexoelectric characterstics. Top panel of Fig. 1 visualizes the cone formation and the localized generation of voltage in graphene sheet under indentation.

WP2: Flexoelectricity in nanostructures

The physical properties of nanostructures (nanotubes, nanocones and nanosprings) and the structural parameters are strongly correlated. We deeply investigate the nanostructure flexoelectric response by varying the nanotube length, nanotube radii, the

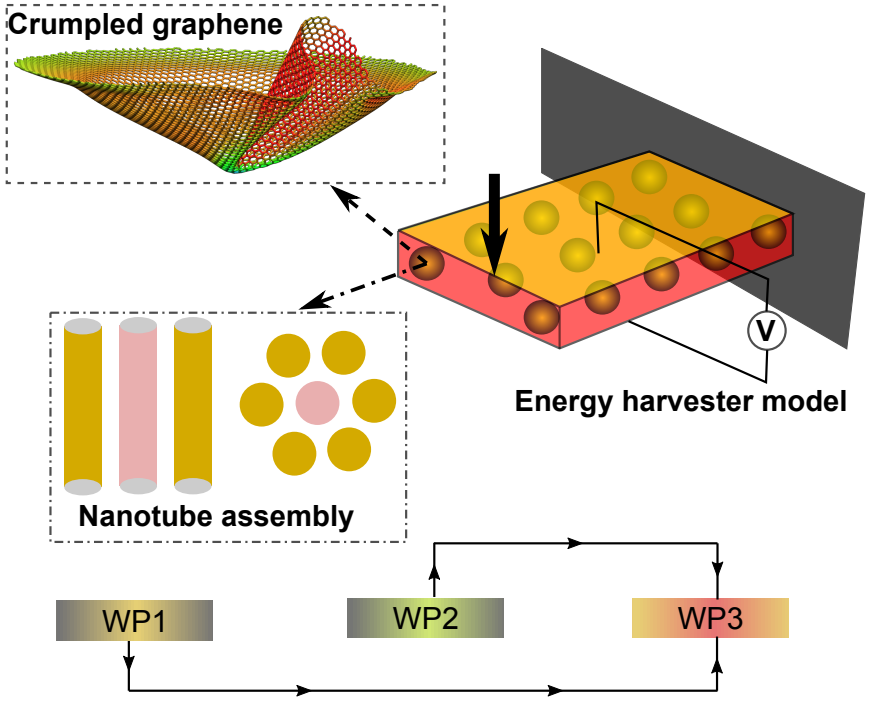

Figure 1: *Schematic of the flexoelectric energy harverster model with nanoscale constituents like crumpled graphene or nanotube assembly.*

apex angle of nanocone, and parameters associated with nanostrucre assembly. The simulation methodology used in the 2D materials is applicable to explore the nanostructures. The bootom panel of Fig. 1 shows the schematic assembly of nanotubes in axial and radial view. Tensile, torsional and shear deformations in higher scale are going to perform to avail the flexoelectric effect.

WP3: Macroscale flexoelectric models

The macroscale model with a continuum approach helps to realize the device scale energy-related applications. Such modeling is dependent on the internal energy density functions involving strain energy, electrostatic energy, and higher-order contributions. Fig. 1 shows the schematic energy harvester model consisting of largely deformed nanoscale 2D materials or nanostructure assemblies. The corresponding input material properties are derived from the nanoscale models. The aim is to estimate the actual voltage/energy generated from this harvester model with the nanoscale constituents.

The computational complexity of the simulation models that we handle requires access to high-performance computing for the following reasons. (I) We are interested to study the large-scale crumpling deformations for the 2D materials to avail the effect of flexoelectricity. (II) A significant number of studies in the structural parameters need to perform to investigate the nanostructure flexoelectricity, which requires many computational resources. (III) The development of machine learning potentials requires hundreds of snapshots from the ab-initio MD simulations. (IV) We need to process large-sized files during the progress of simulations.

WWW

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More Information

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