Micro/Nano-Sized Piezoelectric Structures Analyzed by Strain Gradient Theory

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Abstract: In recent years, a special attention has been directed to the investigation of the relations between the macroscopic material behaviour and its microstructure. For most of the analyses of composite structures, effective or homogenized material properties are used, instead of taking into account the individual component properties and geometrical arrangements. The effective properties are usually difficult or expensive to measure and in the design stage the composition may vary substantially, making frequent measurements prohibitive. Hence a lot of effort has been devoted into the development of mathematical and numerical models to derive homogenized material properties directly from those of the constituents and from their microstructure.

Piezoelectric metamaterials, in which the piezoelectric response of the materials originates from their special geometries or structures and flexoelectricity have been proposed in recent years and the concept can provide a solution for this issue in conventional piezoelectrics [1,2]. Generally, piezoelectricity is observed in materials with noncentrosymmetric crystal structures. However, by exploiting flexoelectricity, the electromechanical coupling defined as the generation of electric polarization by a strain gradient (direct effect) or stress by an electric field gradient (converse effect) in solid dielectrics, even a centric material can exhibit a piezo-electric-like response if the material has special geometries or structures to convert the applied stress into a strain gradient or electric potential into an electric field gradient. The polarization vector in natural piezoelectric material is related to the second order strain tensor through the third order piezoelectric material property tensor. Tensor transformation properties require that under inversion-center symmetry, all odd-order tensors vanish. Thus, most common crystalline materials are not piezoelectric if their structure is centrosymmetric. Physically, however, it is possible to visualize how a non-uniform strain or the presence of strain gradients may potentially break the inversion symmetry and induce polarization even in centrosymmetric crystals [3-5]. Then, one can write

$$P_i \approx f_{ijkl} \varepsilon_{jk,l} ,$$

where f_{ijkl} are the components of the so-called flexoelectric tensor. While the piezoelectric property is non-zero only for select materials (noncentrosymmetric), the strain gradient-polarization coupling (i.e., flexoelectricity tensor) is in principle non-zero for all (insulating) materials. This implies that under a non-uniform strain, all dielectric materials are capable of producing a polarization. The flexoelectric effect has been observed by the non-uniform straining of a graphene nanoribbon, which is a manifestly non-piezoelectric material [6] (Fig. 1).

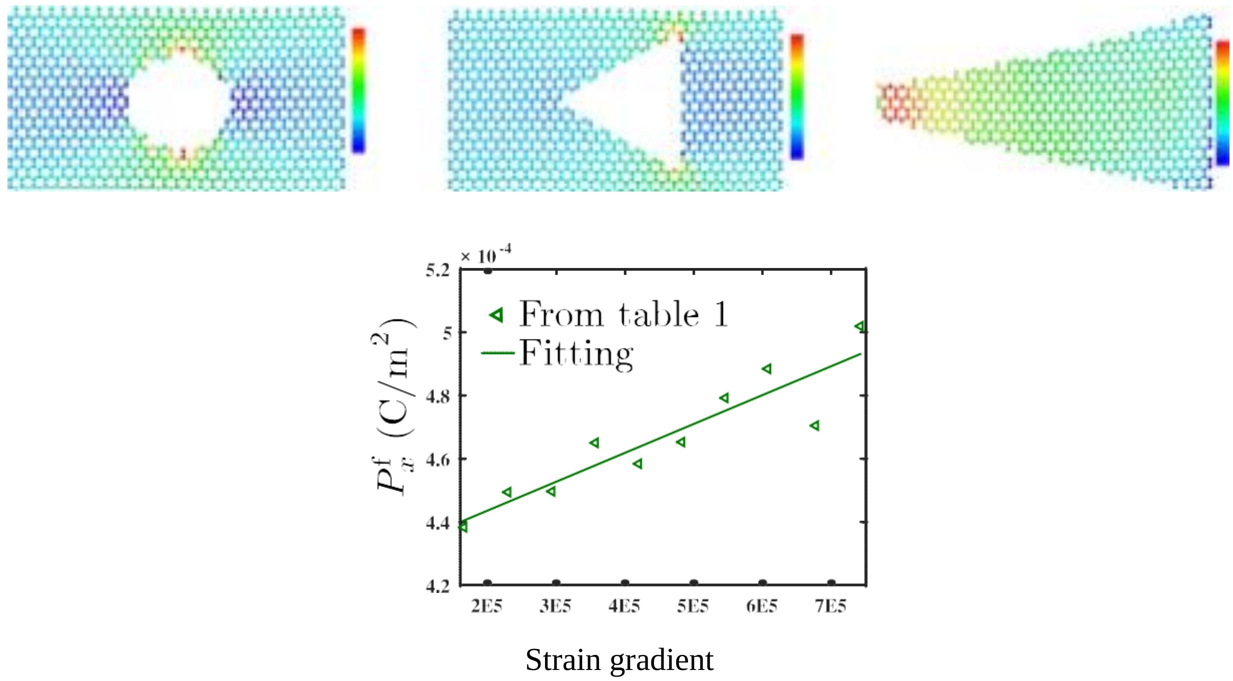

Figure 1: Variation of polarization vector with strain gradient on graphene

The length scales must be “small” since this concept requires very large strain gradients and those for a given strain are generated easily only at the nanoscale. The presence of strain gradients can be realized by differences in material properties at the interfaces of the materials, which result in the presence of strain gradients even under a uniform stress. Those gradients will induce local spatially varying polarization due to the flexoelectric effect. Thus, the artificially structured material will exhibit an electrical response under uniform stress, behaving therefore like a piezoelectric material.

Structural health monitoring (SHM) is especially important for high-performance structures, where failure would lead to disasters, such as nuclear waste containment structures, dams and bridge decks. About 70% of the damage discovered in metallic structures resulted from fatigue cracks. It requires developing sensing method for in-situ monitoring of the onset and growth of cracks at the early stage, especially near the severe strain gradient fastener areas is of growing interest. At present, existing sensing technology (e.g., strain gauges, accelerometers, linear voltage displacement transducers) is not effective for monitoring damage because of its limited sensitivity, bandwidth, and accessibility to the hidden localized areas, let alone damage initiation and progression. Recent research progress on flexoelectricity (FE) suggests a new type of sensors - strain gradient sensors (SGS), which enable highly sensitive detection of strain gradient - the most sensitive measurement near the localized damage location.

For optimal design of devices with flexoelectric properties and in the computational homogenization procedure it is needed to analyse general boundary value problems. It is also well-known that classical continuum mechanics neglects the interaction of material microstructure and the results are size-independent. To overcome intrinsic limitations of classical elasticity, the atomistic models have been developed to micro-scale phenomena in materials. Extremely high requirements on computer memory in atomistic models lead to development multiscale approaches where atomistic and continuum subdomains are bridged. Due to intrinsic heterogeneities in the atomistic-continuum coupling there are some unphysical phenomena observed especially for time-dependent problems. The other alternative is to apply *advanced continuum theories* to account intrinsic length scales for materials. In the gradient theory the strain energy density of a solid depends on the higher order strain gradients too.

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