SASPRO 2
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Modeling of multi-physical phenomena in composite materials

Flexoelectricity

It is well known that piezoelectricity is observed only in materials with non-centrosymmetric crystal structure (Majdoub et al. 2008). In piezoelectric materials a uniform mechanical strain can induce an electric polarization and conversely, a uniform electric field can cause mechanical deformations. However, a non-uniform strain or the presence of strain gradients may potentially break the inversion symmetry and induce polarization even in centrosymmetric crystals (Tagantsev 1986), (Tagantsev et al. 2009), (Maranganti et al 2006). Then, the polarization is proportional to the strain gradients. This effect is called as the flexoelectricity. It is an electro-mechanical 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 atomic structure of material can exhibit a piezo-electric-like response. Then, the flexoelectricity is found to be a universal electromechanical coupling, observed in all dielectrics (Deng et al., 2020). The experimental observations supported the existence of flexoelectric effect in solids (Harris, 1965, Ma and Cross 2001, 2006). The flexoelectric effect is small in large structures, however, it may become significant or even dominant at the nanometer scale. This effect has been observed in a graphene nanoribbon (Dumitrica et al. 2002), (Chandratre and Sharma 2012) and a thin layer Starkov and Starkov (2016) under a nonuniform strain. The flexoelectricity can be utilized also for energy harvesting applications (Jiang et al. 2013, Deng et al. 2014, Faroughi et al. 2019). A review of the theoretical development and experimental progress in flexoelectricity with the future directions for research on flexoelectricity can be found in work (Wang et al. 2019).
Flexoelectricity is also important for a special class of soft materials: biological membranes (Deng et al. 2014). An experimental evidence of flexoelectricity in biological membranes was supported by Brownell et al. (2003). However, the mechanisms of flexoelectricity in polymers is still unclear (Baskaran et al., 2011, 2012; Chu and Salem, 2012). Maybe future atomistic modeling can explain basic unclear mechanisms. The flexoelectricity has been observed also in thermotropic liquid crystals (de Gennes, 1974, Eber and Buka, 2012).

For nano-sized flexoelectric structures it is needed to apply the gradient theory, where governing equations are partial differential equations (PDE) of the fourth order. To solve the flexoelectric problems with strain- and electric intensity vector-gradient effects, several numerical calculation methods are developed, such as moving least square (MLS) (Sladek et al., 2013), meshfree formuation method (Abdollahi et al., 2014, 2015), isogeometric analysis (IGA) (Thai et al., 2018; Nguyen et al., 2018, 2019; Liu et al., 2019), hierarchical B-spline method (Codony et al., 2019), and finite element method (FEM) (Yvonnet and Liu, 2017; Sladek et al., 2018; Amanatidou and Aravas, 2002; Mao and Purohit, 2016; Deng et al., 2017, 2018). Among all the numerical methods presented above, FEM is a powerful computational tool to the general boundary-value-problem (BVP) with a complex geometry. However, the conventional FEM can't be used to study the flexoelectricity due to the strain- and electric intensity vector-gradient effects, where the second derivation of the primary fields (displacement and electric potential) is needed.

There are two modified FEMs to solve this problem in published papers. The first way is to use C^1 continuity element. For example, Yvonnet and Liu (2017) have applied C^1 Argyris triangular elements for soft flexoelectric solids at finite strains. Sladek et al. (2018) have developed conforming elements with C^1 continuity, where each node has 9 degrees of freedom (6 mechanical quantities, electric potential, and two potential gradients) for flexoelectric 2-D problems. The C^1 continuous element is established by using higher order shape functions, and it is very difficult to develop C^1 elements for 3-D problems. Another way to solve the gradient problem is using mixed finite element methods (MFEM). The way based on the MFEM formulation seems to be more convenient, where the C^0 continuous elements are utilized. Following the works of Amanatidou and Aravas (2002) for the mixed FEM in gradient theory of elasticity, Mao and Purohit (2016) constructed a MFEM formulation for flexoelectricity with extra nodal degrees-of-freedom (DOF) for polarizations and developed a 2-D element to solve general BVPs. Latter, Deng et al. (2017, 2018) developed a MFEM with strain gradient and flexoelectricity and extended it to 3-D flexoelectricity problems.

Novel gradient theory for thermoelectric materials

The need to replace the traditional way of electricity production by fossil fuel combustion via green technology is very practical and important. Thermoelectric materials have the potential to convert waste heat directly into electricity through the phenomenon called the Seebeck effect (Callen, 1960; Nagy and Nayfeh, 2000; Minnich et al., 2009; Bies et al., 2002). Despite this potential, thermoelectric materials have not been utilized for production of electricity because of their low efficiency. High thermoelectric efficiency requires a high electrical conductivity, low thermal conductivity and high Seebeck coefficient. A low thermal conductivity ensures sustained large temperature gradients required for generation of a large voltage. It is difficult to satisfy these requirements simultaneously in a single-phase material (Nolan et al., 1999). Therefore, substantial efforts have been devoted to developing high performance thermoelectric composites (Alboni et al., 2008; Cao et al., 2008) and enhancing the thermoelectric properties via varying channels (Sun et al., 2019; Zheng et al., 2019; Wu et al., 2019, Huang et al., 2019; Moshwan et al., 2019; Diez et al., 2020; Kim et al., 2020) for possible nano energy applications (Noyan et al., 2019; Tsao et al., 2019). In terms of micromechanics, Yang et al. (2015) developed an asymptotic homogenization theory for three-dimensional (3D) thermoelectric composites. They used the classical continuum model and implemented it into finite element simulations. A new generation of thermoelectric materials requires a fundamental understanding of the coupled carrier transport involved. In nanotechnology it is possible to reduce thermal conductivity without affecting the electrical conductivity. For instance, optimal thermoelectric properties in nano-structures with particles, wires, or interface architectures were demonstrated (Hochbaum et al., 2008; Boukai et al., 2008). Dominant heat transfer by phonons in nano-sized structures could lead to the reduction of thermal conductivity due to scattering (Stojanovic et al. 2010).

Nanoscale systems are very complex (Majumdar, 1993) and a generalized continuum model based on the nonlocal expression of the heat flux on the temperature gradients (Allen, 2014) is needed. This model could be also utilized for simulations of heat transfer via molecular dynamics (MD). Majumdar (1993) showed that in the microscale regime, heat transport by lattice vibrations or phonons can be analyzed as a radiative transfer problem. Yu et al. (2016) showed that introducing a spatial size effect into the governing equations for heat transfer can explain the incorrect results obtained by classical thermal wave models. Challamel et al. (2016) developed a nonlocal Fourier's law, and applied it to the heat conduction of one-dimensional (1D) and two dimensional (2D) thermal lattices. That model is similar to the differential nonlocal model of Eringen for mechanical interactions. The nonlocality is similar for both thermal and mechanical behaviors and the same length scales were used there for both phenomena. The model with spatial size effects was further applied to nonlocal thermoelasticity using Eringen's nonlocal theory (Yu et al., 2015). Recently, Sarkar (2020) established a nonlocal heat conduction theory of generalized thermoelasticity. Numerical results showed that thermal nonlocal parameters may become a new indicator according to its ability of conducting the thermal energy in solids. Filopoulos et al. (2014a,b) considered the thermoelastic problem within generalized termoelasticity using assumptions of gradient elasticity and non-Fourier heat transfer.

The goal of this work is to develop a novel advanced continuum model for heat transfer considering the size effect occurring in nano-sized structures. From MD simulations, it is known that phonon transport in nanostructures reduces the thermal conductivity. Because the phonon size is comparable with the nano-structure dimension, it is necessary to consider the size effect in the advanced continuum model for heat transfer. The classical Fourier heat conduction model is not sufficient. It is known that nonlocal models for the constitutive relationships lead to an explanation on the size effect and a special treatment of the involved integral kernel makes the convolution integral formulation equivalent to the differential one (e.g. Lazar and Polyzos (2015) for the gradient theory of elasticity). In this paper, we extend the classical theory of thermoelectricity to the generalized nonlocal theory by introducing higher-order derivatives of temperature and higher-grade heat flux.

Boundary-value problems for coupled fields and higher-order derivatives in governing equations are very complex, and analytical solutions are generally not available. Therefore, it is necessary to have a powerful computational tool to solve the general boundary-value problems. The finite element method (FEM) is often convenient for this purpose and it has been applied for many similar problems (Sladek et al., 2017, 2019). The present approach is the first effort to solve this multi-physical problem including size effects in heat transfer. In this study, the second spatial derivative of temperature is considered in the constitutive equation of the higher-order heat flux for a coupled thermo-electric problem. Nano-sized thermoelectric material structures require consideration of the size effect in real and practical modelling. The variational principle is applied to derive the finite element equation for a 2D thermoelectric boundary-value problem. Due to the higher-order derivatives involved in this new gradient theory, C^1-continuous elements are required to guarantee the continuity of the derivatives at element interfaces. Since this is difficult, a mixed FEM formulation is developed here. C^0 continuous interpolation is independently applied to the temperature and its gradients. For modelling the electric field, it is sufficient to use the standard C^0 elements. The constraints between the temperature and its gradients are satisfied at cleverly chosen internal points in the elements (Bishay et al., 2012; Dong and Atluri, 2011).

Publishing activity, especially that of the last five years

Prof. Jan Sladek has published 497 refereed papers and 6 monographs. His research works are cited more than 9159 times (see Google Scholar, http://scholar.google.com/citations?user=EuDw2JcAAAAJ&hl=en) with Hirsh index H=50 and in WOS H=40.