



Surface waves in hexagonal micropolar dielectrics



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ABSTRACT

The propagation of surface waves on a dielectric half-space with hexagonal symmetry is studied on the basis of a recent modification of the micropolar theory of electroelastic continua. The model connects electric polarization to macro and micro-displacements via dipole and quadrupole densities due to the charge distribution in the continuum particle. The differential system derived in the linear wave problem accounts for coupling of acoustic modes with micro-rotational modes referred to polaritons. Bleustein–Gulyaev (BG) and Rayleigh waves are allowed in the half space and are shown to satisfy dispersion laws very similar to those obtained in the past from a phenomenological continuum theory of ferroelectrics. All the surface modes are dispersive and involve polarization via the microrotation gradient. The results prove the effectiveness of the present approach in order to represent electro-elastic coupling in dielectrics. The classical BG wave problem is recovered if microrotation gradient is neglected in the constitutive assumptions but the resulting mode is again dispersive. A similar reduction to the classical Rayleigh wave of linear elasticity allows for a flexoelectric contribution to polarization.

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1. Introduction

Past and recent developments in continuum mechanics of electromagnetic solids have been characterized by a relevant effort to account for various electromagneto-elastic couplings in dielectric, ferroelectric and ferromagnetic media. The most common theories exploit polarization and magnetization as field variables introducing suitable constitutive assumptions. Concerning with dielectric and ferroelectric media, effective models have been developed which account for polarization gradients in their constitutive settings and polarization inertia dealing with dynamical problems (Maugin and Pouget, 1980; Mindlin, 1968, 1972). These theories have been supported by the analysis of atomic interactions in lattice dynamics models (Askar et al., 1970; Pouget et al., 1986a, 1986b) and represent a theoretical basis for the description of a great variety of static and dynamic problems (Eringen and Maugin, 1990; Maugin, 1988).

A different approach to electro-elastic interactions follows from the micromorphic theory of elastic continua (Eringen and Şuhubi, 1964a, 1964b) where additional degrees of freedom are introduced to account for the internal structure of the continuum particle. The usual extensions of this model to electromagnetic media essentially introduce constitutive equations for polarization and magnetization in terms of micro-strain measures

(Eringen, 1999, 2003; Lee et al., 2004). One of the limitations to the applicability of this approach arises from the occurrence of additional, a priori unknown, coupling coefficients, yet beside the enhanced number of constitutive parameters of the purely elastic case. A modification of micromorphic electromagneto-elasticity has been recently suggested in which polarization and magnetization are expressed in terms of internal variables via electric multipoles arising from the charge micro-density (Romeo, 2011, 2012a). The advantage of this approach consists in avoiding additional constitutive assumptions, allowing for a consistent micromorphic model of electroelastic coupling. This coupling arises from the balance equations where the electromagnetic force and couple are directly related to the macro and micro-strain. As in the purely elastic theory, the accuracy of the model depends on the number of degrees of freedom in the microstructure but the electroelastic mechanisms in both elementary or complex models are equivalent to those derived by known evolute phenomenological theories. In particular, the linear micropolar reduction of our model accounts for electroelastic effects just explained by the polarization gradient theories (Mindlin, 1968; Romeo, 2012b).

The aim of the present work is to investigate the consequences of this version of micropolar electro-elasticity to the propagation of surface waves on a dielectric half-space with hexagonal material symmetry. The problem is analogous to those investigated by Pouget and Maugin (1981a, 1981b), concerning Bleustein–Gulyaev (BG) waves and Rayleigh waves in a ferroelectric half-space with material symmetry induced by the intrinsic polarization. We extend the analysis to a dielectric solid focusing to its natural

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piezoelectric properties and assuming, for simplicity, no intrinsic polarization.

The governing equations of the present continuum model are summarized in Section 2 where simplified constitutive assumptions are chosen for the Cauchy stress and the couple stress. Here the dependence on microrotation and its gradient is crucial to account for coupling of acoustic and internal rotational modes (polaritons). The general boundary value problem is formulated in Section 3 and its decoupling into subsystems involving respectively, sagittal and non-sagittal parts of the mechanical displacement is achieved exploiting the material symmetry and a suitable representation of displacement and microrotation. The pertinent expressions for polarization \mathbf{P} in each subsystem are given, showing that the components P_1 and P_2 belonging to the sagittal plane depend only on the microrotation, while P_3 also depends on strain gradient components.

Looking for plane wave solutions, the BG and the Rayleigh problems are solved respectively in Sections 4 and 5 using standard techniques. Both cases of free and grounded surfaces are considered in determining the dispersion law for BG waves and the dependence of mechanical and electric fields on the depth in the half-space is given. Concerning with Rayleigh waves we show that, although in absence of acoustic–polariton coupling the solution reduce to the classical elastic result, the strain gradient contribution to P_3 persists and represents a (not properly piezoelectric) term induced by the dilatational part of the mechanical deformation.

The results are illustrated by numerical examples on wurtzite crystals and show a substantial agreement with the phenomenological continuum model by Pouget and Maugin (1981a, 1981b). The last section is devoted to a comparison of the present results on BG waves with the classical one. Here we show that a reduction to the classical solution can be achieved ignoring microinertia and the constitutive dependence on microrotation gradient. However, the corresponding solution keeps on a dispersive character, showing an irreducible dependence of the electromechanical coupling factor on frequency in BG waves.

2. Preliminaries on a micropolar model for dielectrics

In some previous papers (Romeo, 2011, 2012a, 2012b), we developed a micromorphic model of electro-magneto-elastic continua based on the representation of electromagnetic forces and couples in terms of electric dipoles and quadrupole densities. Concerning with dielectric elastic solids, under the quasi-electrostatic assumption, the balance equations and the Gauss' law for a micropolar continuum can be written in the following form (see Romeo, 2012b)

$$\begin{aligned} \rho \ddot{\mathbf{u}} &= \nabla \cdot \mathbf{T} - (\mathbf{p} \cdot \nabla) \nabla \varphi - \frac{1}{2} (\mathbf{Q} \nabla) [\nabla (\nabla \varphi)] \\ \rho \mathbf{J} \ddot{\boldsymbol{\phi}} &= \boldsymbol{\tau} + \nabla \cdot \boldsymbol{\mu} + \mathbf{p} \times \nabla \varphi + (\mathbf{Q} \nabla) \times \nabla \varphi \\ \nabla \cdot (\mathbf{P} - \nabla \varphi) &= 0 \end{aligned} \quad (2.1)$$

where \mathbf{u} , $\boldsymbol{\phi}$ and φ denote, respectively, the mechanical displacement, the microrotation vector and the scalar electric potential. The Cauchy stress tensor \mathbf{T} and the couple stress tensor $\boldsymbol{\mu}$ account for the contribution of mechanical forces, according to the classical micropolar model, and $\tau_i = \epsilon_{ijk} T_{jk}$ (Eringen, 1999), while the dipole density vector \mathbf{p} and the quadrupole density tensor \mathbf{Q} are responsible for the electric contributions to forces and couples. As usual, ρ denotes the mass density and $\mathbf{J} = (\text{tr} \mathcal{I}) \mathbf{I} - \mathcal{I}$, where \mathcal{I} is the microinertia tensor. The total polarization density \mathbf{P} can be expressed in terms of \mathbf{p} and \mathbf{Q} as

$$\mathbf{P} = \mathbf{p} - \frac{1}{2} \nabla \cdot \mathbf{Q}. \quad (2.2)$$

Within the linear theory, the quantities \mathbf{p} and \mathbf{Q} are given by (see Romeo, 2012a)

$$\begin{aligned} \mathbf{p} &= \mathbf{p}^{(0)} - (\nabla \cdot \mathbf{u}) \mathbf{p}^{(0)} - \mathbf{p}^{(0)} \times \boldsymbol{\phi}, \\ Q_{ij} &= Q_{ij}^{(0)} - (\nabla \cdot \mathbf{u}) Q_{ij}^{(0)} - (\epsilon_{ikl} Q_{kj}^{(0)} + \epsilon_{jkl} Q_{ki}^{(0)}) \phi_l. \end{aligned} \quad (2.3)$$

where $\mathbf{p}^{(0)}$ and $\mathbf{Q}^{(0)}$ denote the intrinsic dipole and quadrupole densities in the unstrained reference configuration. As a consequence, differently from the classical electromagnetic extensions of the micromorphic field theory (Eringen, 1999; Lee et al., 2004) where a constitutive equations is introduced for \mathbf{P} , the total polarization can be explicitly obtained from (2.2) as

$$\begin{aligned} P_i &= p_i^{(0)} - u_{j,j} p_i^{(0)} - \epsilon_{ijk} p_j^{(0)} \phi_k + \frac{1}{2} u_{j,jk} Q_{ki}^{(0)} + \frac{1}{2} (\epsilon_{ikl} Q_{kj}^{(0)} \\ &\quad + \epsilon_{jkl} Q_{ki}^{(0)}) \phi_l. \end{aligned} \quad (2.4)$$

According to both the atomistic and the microcontinuum models of electric polarization (Martin, 1972; Romeo, 2015), a non-vanishing $\mathbf{p}^{(0)}$ accounts for ferroelectricity while $\mathbf{Q}^{(0)}$ characterizes the piezoelectric properties of the dielectric material. The contribution due to $\nabla(\nabla \cdot \mathbf{u})$ in Eq. (2.4) can be ascribed to the flexoelectric part in the multipole expansion of \mathbf{P} , according to Romeo (2015).

The general linear micropolar theory assumes that constitutive equations for \mathbf{T} and $\boldsymbol{\mu}$ came from a strain energy which is a quadratic form of the strain measures $u_{j,i} + \epsilon_{jik} \phi_k$ and $\phi_{i,j}$. Here, in agreement with applications to crystal lattices (Eringen, 1999), we simplify this hypothesis, assuming that coupling terms of these quantities are negligible and write

$$T_{ij} = A_{ijkl} u_{l,k} + \epsilon_{ikh} A_{ijkl} \phi_h, \quad \mu_{ij} = B_{jikl} \phi_{k,l}. \quad (2.5)$$

where the tensors \mathbf{A} and \mathbf{B} comply with the following symmetries

$$A_{ijkl} = A_{klij}, \quad B_{jikl} = B_{klji}.$$

Here we are interested into surface waves polarized along, or orthogonal to, a six-order axis of symmetry of the solid. In particular, we consider the non-centrosymmetric hexagonal class of symmetry 6mm and retain the corresponding non null entries of \mathbf{A} and \mathbf{B} . According to the usual nine-component notation for couple of indices, we get the following independent, non-vanishing entries for \mathbf{A} (see for example Sitotin and Sirotnin and Shaskolskaya (1982))

$$A_{12}, \quad A_{69}, \quad A_{66}, \quad A_{13}, \quad A_{33}, \quad A_{44}, \quad A_{47}, \quad A_{77},$$

and analogous entries for \mathbf{B} . Along with these, the matrix of the tensor \mathbf{J} takes the diagonal form $\mathbf{J} = \text{diag}(J_1, J_1, J_3)$.

Concerning with the dielectric properties, we consider a piezoelectric, non-ferroelectric material assuming $\mathbf{p}^{(0)} = \mathbf{0}$ and the hexagonal structure of wurtzite compounds such as ZnS, CdS, GaN and other wide-bandgap semiconductors. It is easy to check that in this case, accounting for x_3 as the six-fold axis, the charge distribution in the unit cell yields an off-diagonal structure of the matrix $\mathbf{Q}^{(0)}$ with non-vanishing independent entries $Q_{13}^{(0)}, Q_{23}^{(0)}$.

We remark that the assumption $\mathbf{p}^{(0)} \neq \mathbf{0}$ does not allow a direct comparison of the present model with the phenomenological approach to ferroelectrics developed by Pouget and Maugin (1980, 1981a, 1981b) where the non-centrosymmetric structure, and hence piezoelectricity, is induced by the initial polarization $\mathbf{p}^{(0)}$. In fact here, a possible intrinsic polarization simply superimpose to the existing piezoelectric structure of the material.

3. Governing equations for the surface wave problem

Let us assume that the dielectric solid occupy an half-space \mathcal{B} bounded by a plane surface \mathcal{S} and choose a Cartesian coordinate system (x_1, x_2, x_3) with unit vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ such that $\mathbf{e}_2 = \mathbf{n}$ be the inward normal to \mathcal{S} and \mathbf{e}_3 be directed along the six-order

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