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Theoretical investigations on the elastic wave propagation and phonon focusing in AlLi crystal

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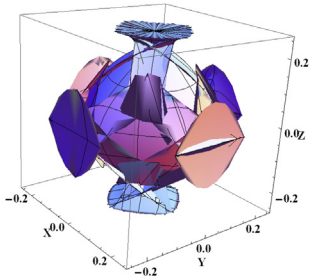
HIGHLIGHTS

- The anisotropic directions of AlLi is [100], [011] and [111] directions.
- The propagation of elastic waves is strongly affected by the elastic anisotropy.
- The phonon caustics "walk along" the maximum direction of elastic anisotropy in AlLi.

GRAPHICAL ABSTRACT



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ABSTRACT

The anisotropy and phonon focusing of AlLi are investigated using ultrasoft pseudopotentials within the generalized gradient approximation correction in the frame of density functional theory. Theoretical calculation of the three dimensional slowness surfaces gives insights into the mixing of longitudinal and transverse modes and shows the origin of the phonon caustics. The results are explained in terms of phonon focusing due to the fact that in elastically anisotropic crystals. The propagation of elastic waves in AlLi is affected by the elastic anisotropy of the lattice.

1. Introduction

In the search for new light-weight materials for aerospace applications, Al–Li alloys have attracted strong attention due to a combination of low density and high stiffness. No other aluminum alloys can compete in that respect [1]. One of the interesting aspects of Al–Li alloys is the occurrence of the stable AlLi phase, which forms as precipitates having the B2 structure [2]. The nature of the bonding has been subject to several discussions [3–7], all of which agree criticizing the picture originally proposed by Zintl and Brauer [8] and Hückel [9]. They [8,9] suggested that in the I–III compounds, the alkali metal transfers its valence electron to the other constituent atom, which then acts as Si in forming a diamond lattice by usual sp^3 bonding. The Al–Li phase diagrams have been widely investigated by the first-principles calculations based on the full-potential linearized augment-plan-wave (FLAPW) method [1,10–12]. Special attention has been paid to the metastable Al_3Li phase and to the mechanical properties of Al-rich Al–Li alloys and the influence of relaxation and vibration entropy are discussed. On the other hand, a Compton scattering is studied for an Al–Li

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disordered alloy single crystal [13], and the elastic properties of Al_{1-x} Li_x random alloys are investigated based on the exact muffin-tin orbital (EMTO) theory within the framework of the single-site coherent potential approximation (CPA) [14], the linear-muffin-tin-orbital (LMTO) method [15], the full-potential linear augmented plane-wave (FLAPW)method [16], and the augmented-spherical-wave(ASW) method [17]. The review on the mechanical properties summaries the microstructure-based micromechanisms of strengthening, of fatigue and fracture as well as of anisotropy in mechanical properties of fatigue and fracture as well as of anisotropy in mechanical properties [18]. The elastic moduli enhancement of Al–Li alloys has been analyzed through the solute (Li, Be, Na, Mg, Ca, and Cu) based on the total-energy calculations [19]. Deformation behavior of binary Al–Li single crystals was investigated with experiment which indicates that the shearing of δ' particles is important in the serrated flow of Al–Li single crystals [20].

Although, excellent progress has been made in understanding these properties in binary AlLi, and significant improvements in the strength and ductility of AlLi single crystal have been achieved through alloying [19]. However, theoretical and practical approaches which are able to address the relationship between the basic issues (such as, nucleation, ductility and dislocations, etc.) and elastic anisotropy of AlLi have not yet been established. Indeed, phonon focusing is a property of all crystals at low temperatures and is strongly affected by the elastic anisotropy of the lattice [21,22].

This effect was first predicted by Taylor, Maris, and Elbaum [23] and the effect was first observed experimentally for the propagation of pulses of thermal acoustic waves in insulators at liquid helium temperatures by Hensel and Dynes [24]. The theory was generalized by Maris, and imaging techniques were later introduced by Northrop and Wolfe [25–28]. However, the relevant researches of AlLi have not been reported, mainly because the solutions of accurate sound velocity in some anisotropic cases are difficult, and the solution of three-dimensional elastic anisotropy is also not easy. Even though the basic mechanical properties, such as flow strength, ductility and the mechanisms of deformation, have been studied extensively in polycrystalline AlLi, a comprehensive characterization of the elastic anisotropy and phonon focusing has not been undertaken for AlLi which required for advanced aerospace structural applications. Phonon focusing is related to the flux of acoustic energy or phonon image (associated with group velocity) in the crystal, the method has been named acoustic-flux imaging or ultrasonic-flux imaging (UFI), regardless of whether the acoustic amplitude, its absolute value, or its square is displayed [29]. One of the most interesting aspects of the technique is that it greatly enlarges the experimental domain for studying elastically anisotropic media. Imaging with heat pulses is generally limited to low temperatures because phonon–phonon scattering restricts the mean free path of high–frequency phonons. In contrast, ultrasonic waves propagate easily through many types of solids at room temperature. Ballistic heat-pulse propagation has also been limited to nonmetallic solids due to the strong scattering of phonons from carriers, whereas ultrasound propagates through metals. Even noncrystalline solids can be transparent to ultrasound, so it is even possible to study elastic anisotropy in composite materials [30]. One promising application of this technique is to alloys and phase transitions. Adapting his ultrasound–imaging apparatus for the transmission mode, Trivisonno [31] obtained the image of alloy crystal of NiAl. The ability to sensitively observe the elastic properties by internal diffraction suggests that this method may be useful for observing phase transitions, such as the Martensitic transition, which has been reported for NiAl with a 63% atomic concentration of Ni at approximately 280 K. In contrast, a comprehensive, intensive, and focused activity should been undertaken within the specific goal of atomic study of AlLi single crystal for the origin of the phonon caustics together with the elastic-wave propagation and the anisotropic elastic properties.

The goal of this paper is to provide a focused, critical discussion and assessment of the phonon-focusing effect arised from elastic anisotropy. In the following section, the physical and elastic properties of AlLi will be discussed, and the slowness surface consisting of three modes of wave propagation will be described.

2. Methodology

The elastic investigation is performed using the CASTEP (Cambridge Serial Total Energy Package) code [32,33]. Vanderbilt-type ultrasoft pseudopotentials (USPP) [34] are employed to describe the electron–ion interactions. The effects of exchange correlation interaction are treated with the generalized gradient approximation (GGA) of Perdew–Burke–Eruzerhof (PBE) [35]. In the structure calculation, a plane-wave basis set with energy cut-off 330.00°eV is used. Pseudo-atomic calculations are performed for $Li2s^1$ and $Al3s^23p^1$. For the Brillouin-zone sampling, we adopt the $10 \times 10 \times 10$ Monkhorst–Pack mesh [36], where the self-consistent convergence of the total energy is at 10^{-7} eV/atom and the maximum force on the atom is blow 10^{-5} eV/Å.

Young's modulus is given by the relation between stress and strain in the direction of the applied load [37]:

$$\varepsilon_{11} = s_{11}\sigma_{11} \text{ or } \sigma_{11} = (1/s_{11})\varepsilon_{11} \tag{1}$$

Here, s_{11} is the elastic-compliance, σ_{11} is stress and ε_{11} is strain in x_1-direction.

Thus, Young's modulus Y in the x_1-direction of a single crystal is represented by the reciprocal of s_{11}. Similarly, the shear modulus G_{12} in the x_1-direction on the x_2-plane or in the x_2-direction on the x_1-plane is given by the reciprocal of s_{66}. When a uniaxial stress σ_{11} is applied in the x_1-direction, Poisson's ratio ν_{12} in the x_2-direction is given by [37]:

$$\nu_{12} = -\varepsilon_{22}/\varepsilon_{11} = -s_{12}/s_{11} \tag{2}$$

Therefore, when the rotational transformation of coordinates is given for the compliance–constant matrix $\{s_{ij}\}$, the reciprocal of Young's modulus, the shear modulus, and Poisson's ratio are given respectively by s_{11}, s_{66}, and $-s_{12}/s_{11}$ for a single crystal with different orientations. The compliance–constant matrix $\{s_{ij}\}$ is a simplified notation of the tensor $\{s_{ijkl}\}$. When the x_1-, x_2-, and x_3-axes are rotationally transformed to the x'_1-, x'_2-, and x'_3-axes, the components of the compliance tensor $\{s'_{pqrs}\}$ after transformations are given by [38]:

$$s'_{pqrs} = \sum_i \sum_j \sum_k \sum_l \alpha_{pi}\alpha_{qj}\alpha_{rk}\alpha_{sl}s_{ijkl}, \left(i,j,k,l = 1,2,3\right) \tag{3}$$

Here, α_{pi}, etc. represent the directional cosines at an angle between the x_i- and x'_p-axes. Then, the compliance–constant matrix $\{s'_{pq}\}$ is obtained for a single crystal with a desired orientation when the tensor $\{s'_{pqrs}\}$ is rewritten in the Voigt notation [39].

Wave propagation in elastic continuum theory is governed by the well-known Christoffel equations [40]

$$\left(\tau_{ij} - \rho v^2\delta_{ij}\right)u_j = 0 \text{ , or } \left(k^2\tau_{ij} - \rho\omega^2\delta_{ij}\right)u_j = 0 \tag{4}$$

where u_j are the displacement components, δ_{ij} is the Kronecker delta, v is the phase velocity, ω is constant frequency, k is the wave vector, and ρ is the density. The Christoffel coefficients are given by