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Structural, elastic and lattice dynamical properties of the alkali metal tellurides: First-principles study



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ABSTRACT

We report a detailed first-principles density functional calculations to understand the systematic trends for crystal structure, elastic and lattice dynamical properties of the anti-fluorite alkali metal tellurides M_2 Te depending from the type of the M cations (M are Li, Na, K and Rb). The calculated equilibrium lattice parameters are in very good agreement with the available experimental data. Single-crystal and polycrystalline elastic moduli and their related properties of the title compounds were calculated via the stress-strain method. The relatively weak values of the calculated elastic moduli demonstrate the weak resistance of these compounds to applied external forces. Phonon dispersion curves throughout the Brillouin zone and corresponding density of states were calculated using the linear response approach. No imaginary phonon modes were found, which indicate the dynamical stability of the examined materials. The atomic displacements at Γ point were determined. Low-frequency dielectric properties and infrared response were investigated.

1. Introduction

The alkali metal chalcogenides M₂Ch [M: Li, Na, K and Rb; Ch: O, S, Se and Te], which crystallize in the face-centered cubic antifluorite (anti-CaF₂-type) structure at ambient conditions [1], possess some interesting physical properties, such as high-temperature properties, fast ionic conduction and wide band gap [2-17]. Owing to these aforementioned properties, the M2Ch materials are potential candidates for several interesting technological applications, such as solidstate batteries [18-20], fuel cells, solid-state gas detectors [21,22] and photo-emissive ultraviolet light materials [23-25]. Among these interesting family members, the alkali metal telluride M₂Te series [M: Li, Na, K and Rb] - the considered compounds - have been the subject of numerous theoretical studies exploring some of their fundamental physical properties. Kikuchiy and co-workers [13] carried out firstprinciples density-functional calculations on the electronic properties of Li₂Te, Na₂Te and K₂Te using the full-potential linearized augmented-plane-wave (FP-LAPW) method. Seifert-Lorentz and Hafner [26] investigated the structural and electronic properties of K₂Te employing a first-principles pseudopotential plane wave (PP-PW) approach. Eithiraj et al. [4] studied the electronic structure of Li₂Te, Na₂Te and K₂Te using the tight-binding linear muffin-tin orbitals (TB-LMTO)

method. Kalarasse and Bennecer [9] explored the elastic properties and lattice dynamics of Na2Te using the PP-PW method. Alay-E-Abbas and co-workers [2,12] studied the structural, electronic and optical properties of the M₂Te [M: Li, Na, K, Rb] series using the FP-LAPW method. Zhang and co-workers [5] investigated the lattice dynamic, thermodynamic and elastic properties of Na₂Te using the PP-PW approach. Bahloul and co-workers [7] studied the structural, electronic and elastic properties of Li2Te employing the PP-PW approach. Zhang and Shi [10] investigated the lattice dynamics, thermodynamics and elastic properties of Li2Te through the PP-PW formalism. In spite of these numerous already performed theoretical studies on the alkali metal tellurides M2Te [M: Li, Na, K, Rb], one can note that a lack of information on some of their physical properties still exists up to now. On one hand, as far as we know, there are no theoretical or experimental investigations of the lattice dynamical, elastic and thermodynamic properties of the K2Te and Rb2Te systems. On the other hand, no study was performed to investigate the systematic trends for the structural, elastic, lattice dynamical and thermodynamic properties of the M₂Te family depending from the type of M elements (M are Li, Na, K and Rb). Recently, first-principles investigations of the lattice dynamical and thermodynamic properties of materials have provided some quite satisfactory results [27-33]. In view of these

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circumstances, in the present paper a systematic first-principles study of the structural, elastic and lattice dynamical properties for the M_2 Te [M: Li, Na, K and Rb] series was performed using the pseudopotential plane wave method within the generalized gradient approximation.

2. Computational details

All our first-principles calculations were performed within the framework of the density functional theory (DFT) and density functional perturbation theory (DFPT) using the pseudopotential planewave (PP-PW) method as implemented in the CASTEP (Cambridge Total Energy Package) code [33]. The electronic exchange and correlation potentials were described using the generalized gradient approximation GGA-PBEsol [34] (it is termed also GGA08), which has been specially developed to improve the description of the exchangecorrelation potential in solids. Norm-conserving pseudopotentials [33] were used to describe the interaction potential between the valence electrons and the nucleus and frozen electrons. A plane-wave basis set cut-off of 800 eV and a 15 × 15 × 15 Monkhorst-Pack scheme *k*-points grid [35] for the integration over the Brillouin zone (BZ) were applied to ensure sufficiently accurate total energy calculations. The optimized lattice parameters were calculated by using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) minimization algorithm [36]. The optimized geometry was performed with the following convergence criteria: (i) the total energy difference between two consecutive iterations were smaller than $5.0 \times 10^{-6} \text{ eV/atom}$ and (ii) the stress was smaller than 0.02 GPa. The single-crystal elastic constants C_{ii}s were determined from first-principles calculations by applying a set of given homogeneous deformations with a finite value ε and calculating the resulting stress with respect to optimizing the internal atomic freedoms. The Cijs were obtained via linear fittings of the stress-strain curves computed from accurate ab initio calculations [33]: the elastic stiffness tensor is related to the stress tensor and the strain tensor by Hooke's law. To determine the three independent elastic constants C_{ij} s of a cubic system, namely C_{11} , C_{44} and C_{12} , one strain pattern with nonzero ε_{11} and ε_{23} was used. The maximum strain amplitude was set at 0.003. The lattice vibrational properties, namely the phonon dispersion curves, density of phonon states, dielectric tensors and thermodynamic properties were calculated using the linear response method within the density functional perturbation theory (DFPT) [37]. The dielectric tensor and the longitudinal-optical/transverse-optical (LO-TO) splitting are used to calculate the frequencydependent optical properties in the infrared region (low-frequency region). The phonon frequencies were computed on a $10 \times 10 \times 10 q$ points mesh in the BZ.

3. Results and discussion

3.1. Structural properties

At ambient conditions, the M2Te [M: Li, Na, K, Rb] compounds crystallize in the anti-CaF₂-type structure, space group $Fm\overline{3}m$ (no. 225), with four formula units (Z = 4) per unit-cell [1]. Fig. 1 depicts one unitcell of the K₂Te compound as a representative of the M₂Te (M: Li, Na, K, Rb) series. The Te atom occupy the Wyckoff position 4a(0, 0, 0); the corner and face-centered positions, and the alkali metal atom M are located at the Wyckoff position 8c (0.25, 0.25, 0.25), filling the octahedral holes. Therefore, each Te atom is surrounded by eight M atoms and each M atom is attached to four Te atoms as it is shown in Fig. 1 by polyhedrons. Before performing calculations to obtain the elastic constants and lattice vibrational properties of the considered compounds, their equilibrium lattice parameters (a_0) were determined using the above-mentioned settings. Table 1 presents the obtained results along with the available theoretical and experimental data in the scientific literature. Our obtained values for all considered alkali metal tellurides are in excellent accord with the measured ones. Our



Fig. 1. The centered-faced cubic anti-fluorite Ca_2T -type conventional unit-cell for the K_2Te crystal as representative for the M_2Te [M: Li, Na, K and Rb] series.

calculated values differ from the corresponding measured ones [1,2,26,38] by less than 0.4%, 0.6%, 1.0% and 0.7% for Li₂Te, Li₂Na, Li₂K and Li₂Rb, respectively. Table 1 shows also a good agreement between our results and those from earlier calculations [2,4,5,7,9,10,26]. The lattice parameter a_0 increases with increasing atomic number Z of the alkali metal atoms, i.e., $a_0^{Li_2Te} < a_0^{Na_2Te} < a_0^{K_2Te} < a_0^{Rb_2Te}$. This trend can be attributed to the increase of the atomic radius (R) of the alkali metal atom M in the M₂Te series (M: Li, Na, K, Rb) with the increase of their atomic number Z, i.e., R(Li) < R(Na) < R(K) < R(Rb). In order to obtain the bulk modulus B and its pressure derivative B' values, the calculated primitive-cell volumes (V) as a function of pressure for each considered compound are fitted to the Murnaghan equation of state (EOS) [39]. The obtained values for B and B', listed in Table 1, are in good agreement with the reported data in the scientific literature. The bulk modulus value decreases when going in the following sequence $Li_2Te \rightarrow Na_2Te \rightarrow K_2Te \rightarrow Rb_2Te$, which is in accordance with the Cohen's approximation $B \sim V^{-k}$ [40].

3.2. Elastic constants and related properties

The single-crystal elastic constants C_{ij} are among the most important parameters that characterize the physical properties of crystals. From a practical point, the elastic constants measure the resistance of a solid to an external applied macroscopic stress and their abilities to recover and regain their original shape after stress ceases. Thus, they provide important information regarding the strength, ductility and hardness of materials. In addition, some macroscopic elastic moduli such as the bulk, Young and shear moduli and Poisson's ratio, which characterize the mechanical properties of solids, can be obtained from the C_{ii} s. From a fundamental viewpoint, the elastic constants are the second derivative of the total energy with respect to strain. Therefore, from the elastic constants, one can derived valuable information on the mechanical stability and the stiffness of the binding between adjacent atomic planes, sound wave velocities, anisotropic character of the bonding, Debye temperature and so on. The computed single-crystal elastic constants C_{11} , C_{12} and C_{44} for the examined systems are quoted in Table 2 as well as available values from other theoretical reports [5,7,9,10] for comparison. The obtained data allow us to make the following conclusions:

 No experiments have been conducted out to measure the singlecrystal elastic constants C_{ij}s to be compared with our obtained Download English Version:

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