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Short communication

Theoretical investigation of mechanical and thermal properties of MPO_4 (M = Al, Ga)

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Abstract

Minimum lattice thermal conductivities and mechanical properties of polymorphous MPO_4 (M = Al, Ga) are investigated by first principles calculations. The theoretical minimum thermal conductivities are found to be 1.02 W (m K)$^{-1}$ for α-$AlPO_4$, 1.20 W (m K)$^{-1}$ for β-$AlPO_4$, 0.87 W (m K)$^{-1}$ for α-$GaPO_4$ and 0.88 W (m K)$^{-1}$ for β-$GaPO_4$. The lower thermal conductivities in comparison to YSZ can be attributed to the lattice phonon scattering due to the framework of heterogeneous bonds. In addition, the low shear-to-bulk modulus ratio for both β-$AlPO_4$ (0.38) and β-$GaPO_4$ (0.30) is observed. Our results suggest their applications as light-weight thermal insulator and damage-tolerant/machinable ceramics.
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Keywords: Ceramic; Thermal conductivity; Mechanical properties; First principles calculations

1. Introduction

Polymorphous MPO_4 (M = Al, Ga) which are isomorphous to SiO_2, crystallize in both α- and β-quartz like structures. As shown in Fig. 1, both α- and β-quartz forms of MPO_4 consist of corner linked $(MO_4)^{5-}$ and $(PO_4)^{3-}$ tetrahedra. The α-quartz type MPO_4 has the $P3_121$ space group while the β-quartz type has the $P6_422$ space group. As candidates of the piezoelectric crystal, various properties of MPO_4 (M = Al, Ga) such as optical activity, electro-optical effect and piezoelectricity have been widely studied.[1–3] On the other hand, the mechanism of α–β phase transition has been clarified. The α phase can be derived from the β phase by tilting angle δ, which is 21.2° for $AlPO_4$ and 23.1° for $GaPO_4$, around the hexagonal a-axes.[2]

However, their potential applications as structural materials have not yet been fully understood. Their structures of corner-linked polyhedra combining with heterogeneous bonding strength are typical structural characteristics of damage-tolerant ceramics and thermal insulators, such as $LaPO_4$[4] and $Re_2SrAl_2O_7$.[5] Damage tolerant ceramics can be used as weak interfacial phases in order to allow crack deflection and fiber pull-out in ceramic–matrix composites. Thermal insulators are widely used as thermal and environmental barrier coatings.[6–7] In comparison to other well studied damage tolerant ceramics and thermal insulators, MPO_4 (M = Al, Ga) owns very light-weight. This advantage is of vital importance in aeronautic and aerospace industries. In addition, widely applications of such kind of light-weight materials in transportations and manufactories will help to save energies. While there are few theoretical and experimental studies on the mechanical properties of α-phase MPO_4,[8–9] the mechanical properties of β-phase and thermal conductivities of both α- and β-MPO_4 are still not well understood. Such lack has blocked their potential applications as structural materials as well as insulators for thermal management.

In this work, state-of-the-art first-principles calculations were performed on α- and β-quartz forms of MPO_4. We first calculate the equilibrium crystal structure, elastic constants, bulk modulus, shear modulus, and Young's modulus of MPO_4. Then, the theoretical minimum lattice thermal conductivity (κ_{min}) of each ternary compound is calculated by combining first principles calculations with Debye model, which has proven

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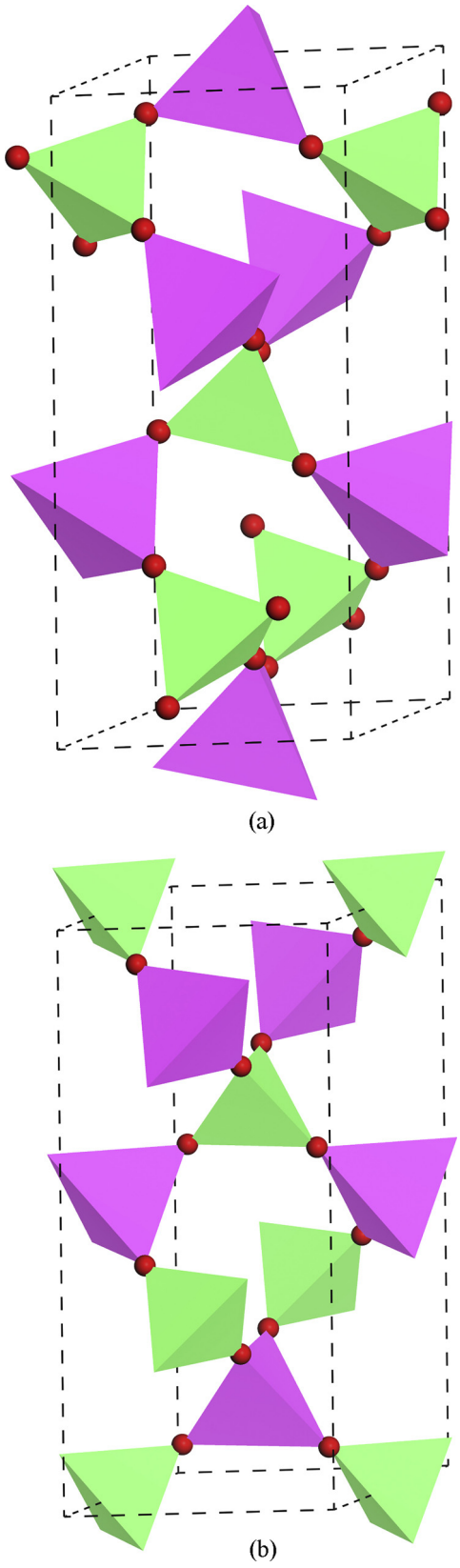

Fig. 1. Crystal structures of (a) α- and (b) β-MPO$_4$ (M = Al, Ga). $(MO_4)^{5-}$ and $(PO_4)^{3-}$ tetrahedral are purple and green, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

to be an efficient and economical way to predict thermal conductivities.[5,10,11] Based on our work, MPO$_4$ is predicted to be a new group of low thermal conductive and/or damage tolerant ceramics. Finally, the effect of heterogeneous bonds on κ_{min} is discussed.

2. Computational methodology

Theoretical investigations were accomplished using the CASTEP code,[12] in which the plane-wave pseudopotential total energy calculation was employed. The plane wave energy cut-off and the Brillouin zone sampling were fixed to 450 eV and $3 \times 3 \times 2$ special k-point meshes, respectively. The electronic exchange-correlation energy was treated under the local density approximations (LDAs).[13] The crystal structures were fully optimized by independently modifying lattice parameters and internal atomic coordinates. The Broyden–Fletcher–Goldfarb–Shanno minimization scheme[14] was used to minimize the total energy and interatomic forces. The elastic coefficients were determined from first-principles calculations by applying a set of given homogeneous deformations with a finite value and calculating the resulting stress with respect to optimizing the internal degrees of freedoms.[15] For α-AlPO$_4$, three positive and three negative amplitudes were applied for each strain component with maximum strain value of 0.5%. However, for β-AlPO$_4$, α-GaPO$_4$ and β-GaPO$_4$, only four amplitudes were applied for each strain component with maximum strain value of 0.3% to avoid the nonlinear stress–strain relationship at ±0.5%. Detailed computational parameters can be found in our previous work, wherein we predicted crystal structure, elastic stiffness, and thermal conductivities of ternary oxides.[10,11]

The lattice thermal conductivity (κ) of a solid can be calculated by

$$\kappa = \frac{1}{3} C_v v_m \Lambda \tag{1}$$

where C_v is the specific heat, v_m is the mean sound velocity and Λ is the phonon mean-free path. At temperatures higher than Debye temperature, the specific heat C_v is close to its temperature independent value of $3k_B$/atom (k_B is Boltzmann constant) predicted by Dulong–Petit equation and the lattice thermal conductivity approaches to the minimum lattice thermal conductivity, κ_{min}.[7] In order to calculate κ_{min}, it was suggested that different atoms in a molecule could be treated as an equivalent atom with a mean atom mass of M/n (M is the molecule mass and n is the number of atoms per molecule) and therefore the minimum Λ is approximated by the average atomic distance.[7] For sound velocity v_m, a standard calculation method used in our previous work[11] is adopted here:

$$v_m = \left(\frac{3(v_s v_l)^3}{2v_l^3 + v_s^3} \right)^{1/3} \tag{2}$$

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