Electron–phonon coupling in APd$_3$O$_4$: $A = \text{Ca, Sr, and Sr}_{0.85}\text{Li}_{0.15}$

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Abstract

Here we have investigated the role of electron–phonon coupling on the Raman spectrum of narrow bandgap semiconductors APd$_3$O$_4$ ($A = \text{Ca, Sr}$) and hole-doped system Sr$_{0.85}$Li$_{0.15}$Pd$_3$O$_4$. Four Raman active phonons are observed at room temperature for all three compounds as predicted by factor group analysis. The lowest energy phonon ($\sim 190/202$ cm$^{-1}$) associated with Pd vibrations is observed to exhibit an asymmetric Fano-like lineshape in all the three compounds, indicating the presence of an interaction between the phonon and the electronic continuum. The origin of the electronic continuum states and electron–phonon coupling are discussed based on our laser power- and temperature-dependent Raman results. We have observed an enhanced strength of electron–phonon coupling in Sr$_{0.85}$Li$_{0.15}$Pd$_3$O$_4$ at low temperatures which can be attributed to the metallicity in this doped compound.

Keywords: electron–phonon coupling, Raman spectroscopy, Fano resonance, Alkaline earth ternary palladates, x-ray diffraction

Supplementary material for this article is available online

(Some figures may appear in colour only in the online journal)

1. Introduction

The interplay between lattice and electronic degrees of freedom is the key factor for various exotic phenomena in condensed matter physics and material science, such as quantum effects in thermodynamics, superconductivity, phonon and electron transport, phonon-assisted light absorption, and temperature-dependent optical properties of materials [1–4]. The electron–phonon coupling (EPC) reinforces the temperature-dependence of electrical resistivity in metals, carrier mobility in semiconductors, and also play a crucial role in materials exhibiting charge density waves as well as in the areas of spintronics and quantum information [5, 6]. On the other hand, semiconductors are the leading materials for next generation technologies to solve challenges in sustainable energy and environmental remediation [7]. Semiconductors with narrower band gap are widely used for infrared radiation detection, optoelectronic and thermoelectric device fabrication [8]. It was realized that the inclusion of EPC was necessary to interpret spectral and transport properties of semiconductors accurately [9]. In a semimetallic or narrow band gap semiconducting system, formation of excitons under suitable conditions may lead to a new exotic ground state, called excitonic insulator (EI) in which the Coulomb interaction and EPC are driving mechanisms [10].

In this context, in general, the nonmagnetic Pd transition metal and its transition metal oxides are receiving enormous attention due to their various ground states with the EPC controlled peculiar properties, owing to their unique crystal structure. For instance, the ground state and properties of Pd transition metal, lattice thermal conductivity of PdCoO$_2$ are well controlled by the EPC [11–13]. The complex palladate oxides with narrow bandgap having significant Pd–4d states around the Fermi level ($E_F$) may allow the system to undergo an insulator to metal transition (IMT) upon hole/electron doping via monovalent/trivalent ion substitution at $A$-site [14–21]. For
example, it was realized in PdO [15], PdPbO₂ [16, 17] and APd₃O₄ (A = Ca, Sr) systems [18–21]. Among all, APd₃O₄ (A = Ca and Sr) systems are potential candidates to explore the vibrational properties, possibility of EPC and IMT due to their unique crystal structure (NaPt₃O₄-type whose ground state and physical properties are driven by EPC [22]) and narrow band gap semiconducting nature (with the electronic bandgap value of 0.25 and 0.22 eV for CaPd₃O₄ and SrPd₃O₄, respectively obtained from transport measurements [23]). On the other hand, it was theoretically predicted that CaPd₃O₄ is a potential candidate for being an EI [24] although experiments suggested that it is unlikely to be [18]. Hence, it is very important to understand phonons and their correlation with electronic degrees of freedom in these systems. APd₃O₄ (A = Ca and Sr) systems may also be suitable for thermoelectric applications such as switching and sensing devices due to their narrow bandgap [17, 21, 23]. Since phonons and/or EPC have intimate relationship with thermoelectric properties, IMT, EI etc [10, 25–27], and to the best of our knowledge, there are no phonon studies on these systems, we consider worth exploring phonons, possibility of EPC and IMT in these systems.

The optical spectroscopy is a powerful technique for investigating electronic and vibrational properties of a variety of systems and has provided extensive information and insights into the properties of solids [28]. For example, the strong EPC manifests itself in the form of asymmetric line shape of phonon mode in Raman or infrared spectrum [29–31], which can be analyzed by using Breit–Wigner–Fano (BWF) interference model. Here, we present the synthesis, crystal structure, and first experimental results of Raman spectroscopic measurements of the ternary palladates Ca₃PdO₄, Sr₃PdO₄ and Sr₀.₈₅Li₀.₁₅Pd₃O₄. The lowest energy phonon of \( E_g/T_{2g} \) symmetry shows the Fano resonance due to EPC. The semiconductor to metal transition is observed by hole doping via Li⁺ substitution at the place of Sr in SrPd₃O₄. The temperature-dependence of asymmetry parameter (1/\( \alpha \)) in all the three systems is in coordination with their electronic properties and band structure. More importantly, our results suggest that the EPC is tunable with chemical substitution and temperature in these systems thus making them potential candidates for various applications.

2. Experimental details

Polycrystalline Alkaline earth ternary palladates APd₃O₄ with A = Ca, Sr, and Sr₀.₈₅Li₀.₁₅ were prepared by solid-state reaction route. High purity chemicals of CaCO₃, SrCO₃, PdO, and Li₂CO₃ from sigma Aldrich were used as starting materials. A stoichiometric mixture of precursors was calcined at 630 °C for 18 h. Sintering was done at 700 °C for a few times with intermediate grindings and pelleting each time. Temperature-dependent powder x-ray diffraction (PXRD) measurements were done by using PANalytical Empyrean x-ray diffractometer with Cu–Kα radiation of wavelength 1.5406 Å attached with Anton Paar TTK 450 heating stage. Raman spectra were collected in the backscattering configuration using a LabRAM HR evolution Raman spectrometer attached to a 532 nm laser excitation source and Peltier cooled charge-coupled device detector. HFS600E-PB4 Linkam stage was used for temperature-dependent Raman measurements.

The phonons have also been calculated using projector augmented wave method implemented in the Quantum Espresso code [32]. The optimization for total energy, lattice parameter, and phonon calculation was done using energy cut-off 150 Ry and 4 × 4 × 4 Monkhorst–Pack grids. The cubic lattice was kept fixed and equilibrium lattice constant of SrPd₃O₄ has been obtained by minimizing the calculated total energy as a function of lattice constant. We have chosen pseudopotentials generated using Perdew–Burke–Ernzerhof (PBEsol) exchange correlation.

3. Results and discussion

Alkaline earth palladates such as CaPd₃O₄ and SrPd₃O₄ crystallize in NaPt₃O₄-type crystal structure. The unit cell structure is drawn using VESTA (visualization for electronic and structural analysis) software [33] and displayed in figure 1(a). In this structure, each divalent Pd ion is coordinated with four O−² ions located in PdO₄ square planes. A-site atom is connected to eight O−² ions forming A06 cubes. The A06 cubes are connected to each other by PdO₄ planes through their edges [22, 34, 35]. PXRD data collected on as prepared polycrystalline samples of APd₃O₄ with A = Ca, Sr, and Sr₀.₈₅Li₀.₁₅ (will be represented now on as CP, SP, and SLP, respectively) are refined by Rietveld method and displayed in figure 1(b). It confirms that powder samples are stabilized in cubic structure with the \( Pm\bar{3}n \) (no. 223) crystal symmetry. Rietveld refined lattice parameters and bond lengths for CP, SP, and SLP are listed in table 1 which are in agreement with the earlier reports [23, 35–37]. The effective A-site radius [38] for SP, SLP, and CP is 1.26 Å, 1.22 Å, and 1.12 Å, respectively, that explains the observed trend (decrease) in the lattice parameters. The Pd−O bond length is similar to that found in PdO crystal (Pd−O = 2.03 Å) where Pd ions lie at the centres of rectangles and oxygen ions at each corner [39]. The Pd ion is divalent in these compounds with the electronic configuration 4d⁸. The 4d energy levels split into \( d_{x^2−y^2}, d_{xz}, d_{yz}, d_{xy}, \) and \( d_{xy}^2−y^2 \) in increasing order of energy due to the square planar configuration (schematic is given in figure S1 in supplementary material https://stacks.iop.org/JPCM/33/105601/mmedia) [40]. The highest energy orbital, \( d_{xy}^2−y^2 \), is empty with a small gap thus making CaPd₃O₄ and SrPd₃O₄ semiconducting in nature [41]. It is important to note here that the electronic structure calculations based on generalized gradient approximations (GGA) do not produce band gap suggesting that the electron–electron correlation plays an important role in these systems. It is GGA + U calculations which produces a small gap for U ~ 4.5 eV (see figure S2 in supplementary material). Other calculations based on hybrid functionals [23] also produce similar gaps in these systems confirming the role of electron correlation. Due to the small gap in these systems thermally- and/or photo- excited carriers can couple to the phonon degree of freedom exhibiting the EPC with varying
Figure 1. (a) Crystallographic unit cell, (b) showing AO$_8$ cube and PdO$_4$ square planes (c)–(e) x-ray diffraction pattern collected at a few temperatures and (f) lattice parameters as a function of temperature for APd$_3$O$_4$ with $A = $ Ca, Sr, and Sr$_{0.85}$Li$_{0.15}$. Error bars in (f) are within the symbol size.

Table 1. Room temperature lattice parameters and bond lengths extracted from x-ray diffraction results.

| Compound          | Lattice parameter a (Å) | Bond lengths (Å) | Pd–O | A–O | A–Pd |
|-------------------|-------------------------|------------------|------|-----|------|
| SrPd$_3$O$_4$     | 5.8277                  | 2.0581 2.5230 3.2530 |
| Sr$_{0.85}$Li$_{0.15}$Pd$_3$O$_4$ | 5.8194                  | 2.0575 2.5199 3.2531 |
| CaPd$_3$O$_4$     | 5.7391                  | 2.0290 2.4851 3.2082 |

Calculated lattice parameter for SrPd$_3$O$_4$ is 5.82 Å.

To further investigate the effect of temperature on crystal structure and lattice parameters, we have performed temperature-dependent x-ray diffraction measurements in the range of 90–400 K. Figures 1(c)–(e) shows the x-ray diffraction patterns collected at a few temperatures for CP, SP, and SLP, respectively. Symbols in figure 1(f) show the temperature dependent lattice parameters obtained from Rietveld refinement of diffraction patterns for all three compounds. Fit using thermal expansion equation [44] as shown by lines in the figure 1(f) suggests no structural phase transition or anomalies in the lattice parameters and all the three compounds exhibit positive thermal expansion in the investigated temperature range (90–400 K).

Figure 2 shows the Raman spectra of APd$_3$O$_4$ (A = Ca, Sr, and Sr$_{0.85}$Li$_{0.15}$) collected at room temperature. According to the factor group analysis, the cubic structure with the Pm3n symmetry leads to four Raman active and five infrared (IR) active phonon modes with irreducible representations.

Γ$_{\text{Raman}} = 2E_g + 2T_{2g}$ and Γ$_{\text{IR}} = 5T_{1u}$ [45]. Four Raman active modes including two ‘$E_g$’ and two ‘$T_{2g}$’ are observed in agreement with the group theory predictions. The experimentally observed phonon frequencies at room temperature and corresponding mode symmetries are compiled in table 2. Our phonon calculations at the Γ’-point of Brillouin zone based on Quantum Espresso support the mode assignments (see table S1 in supplementary material). The mode P0 (E$_{g}^{-1}$) and P1 (T$_{2g}^{-1}$) strength due to the temperature and laser power variations [42, 43].
where

$$\omega$$

are coupled. The BWF model lineshape is given by [31, 46]:

$$I = A \left( \frac{\omega - \omega_P}{1 + \varepsilon^2} \right)^2$$

$$= A \left[ \frac{1}{q} + \frac{(1 - q/\omega_P)}{1 + \varepsilon^2} + \frac{\varepsilon^2}{1 + \varepsilon^2} \right]$$,

(1)

where \(\varepsilon = \frac{2(\omega - \omega_P)}{1 + \varepsilon^2}\) and \(1/q\) is the degree of EPC that describes the departure of the lineshape from a symmetric Lorentzian function. \(A\) is the maximum intensity of the BWF spectra, \(\omega_P\) and \(\Gamma/2\) are the real and imaginary part of phonon self-energy, respectively. In equation (1), the first term \(\left(\frac{1}{q}\right)\) represents a constant continuum spectrum, the second term is for a discrete Lorentzian spectrum while the interference effect between both spectra is accounted by the third term \(\left(\frac{\varepsilon^2}{1 + \varepsilon^2}\right)\). The interference term resembles the ratio between the probability amplitude of the continuum spectrum to that of the discrete spectrum, giving rise to an asymmetric lineshape in the Raman spectrum. The asymmetric Raman lineshape (equation (1)) takes a Lorentzian profile when there is no EPC i.e. when \(\frac{1}{q} = 0\). Figure 3 shows the Raman spectra collected at a few different laser powers using 532 nm radiation. A clear redshift in the peak position and an increase in the asymmetry are observed with increasing laser power. The insets of figure 3 display corresponding Stokes and anti-Stokes spectra collected at the highest laser power used (2.37 mW) which clearly shows that both the Stokes and anti-Stokes spectral shapes are symmetric. As a result of this, the spectra are fitted with BWF lineshape and the corresponding parameters (frequency, linewidth, and asymmetry parameter) are plotted as a function of the laser power as shown in figures 4(b), (d) and (f). The phonon frequency (linewidth) decreases (increases) with increasing laser power while the asymmetry parameter \(1/q\) increases with increasing laser power. The increase in \(\frac{1}{q}\) with laser power is photo-induced effect where photo-excited (and thermally excited due to laser heating at higher powers) carriers couple to the phonons. The corresponding parameters of the mode P1 in the anti-Stokes spectrum also show similar behaviour (not shown here). The redshift in the phonon frequency can be attributed to the laser heating effect. The mode softening and symmetric (Lorentzian) broadening of the phonon modes P2, P3, and P4 can be attributed to the lattice anharmonic effects (see figures S4 and S5 in supplementary material). In order to understand the temperature-dependence

| Mode  | Symmetry | Frequency (cm\(^{-1}\)) |
|-------|----------|------------------------|
|       |          | Cal. | Expt. | Expt. |
| P0    | \(E_g^1\) | 177 | 185\(^a\) | Too weak to be observed | 200\(^a\) |
| P1    | \(T_{2g}^2\) | 193 | 190 | 193 | 202 |
| P2    | Defect-induced Raman-active | — | 508 | 511 | 554 | O |
| P3    | \(T_{2g}^2\) | 512 | 546 | 553 | 592 | O |
| P4    | \(E_g^2\) | 539 | 553 | 556 | 599 | O |

Calculated acoustic/IR active phonon frequencies with \(T_{1u}\) symmetry are 0 [Sr], 151 [Pd], 161 [Pd], 370 [O], and 551 [O] cm\(^{-1}\).

The atoms involved in corresponding vibration are mentioned in the square brackets.

\(^a\)Indicates the weak modes and frequency value is given at 80 K.

| Frequency of Raman active phonons at room temperature. |
|--------------------------------------------------------|
| Space group \(Pm\overline{3}n\) (no.223) and point group \(O_h\) (no.230) |
| Wyckoff positions | Irreducible representations |
| Sr/Ca/Li: 2a | \(T_{1u}\) |
| Pd: 6c | \(E_g + T_{2g} + 2T_{1u}\) |
| O: 8e | \(E_g + T_{2g} + 2T_{1u}\) |

Total irreducible representations \(\Gamma_{\text{Raman}} = 2E_g + 2T_{2g} + \Gamma_{\text{IR}} = 5T_{1u}\).
Figure 3. (a), (c) and (e) The response of the Raman mode P1 collected at a few different laser powers, and (b), (d) and (f) the dependence of Fano asymmetry parameter ($1/q$) as a function of laser power for APd$_3$O$_4$ with $A =$ Ca, Sr, and Sr$_{0.85}$Li$_{0.15}$. The solid lines overlaying the data in (a), (c) and (e) are Fano lineshape analysis. The solid lines in (b), (d) and (f) and their insets are guide to eye. The insets in (a), (c) and (e) show the Stoke vs anti-Stokes spectra at the respective laser powers exhibiting the Fano asymmetry.

Figure 4. Raman spectra (shown for the mode P1) collected at a few temperatures (a), (c) and (e); phonon frequency and linewidth as a function of temperature (b), (d) and (f) for APd$_3$O$_4$ with $A =$ Ca, Sr, and Sr$_{0.85}$Li$_{0.15}$. Green solid lines in (b), (d) and (f) are fitting with anharmonic model (explained in the text). The insets in (a) and (c) show the presence of mode P0 at lowest measured temperature (80 K). of the EPC, as indicated by the asymmetric lineshape of the mode P1, we have collected the Raman spectra in the temperature range of 80–600 K (figure S5 in supplementary material). The temperature-dependence of the remaining phonon modes is given and discussed in supplementary material.

Figure 4 displays the profile for P1 mode at a few temperatures along with Fano fitting (solid lines in figures 4(a), (c) and (e)). The extracted phonon parameters (frequency and linewidth) are plotted as a function of temperature for all the three compounds in figures 4(b), (d) and (f). The mode shows clear redshift in frequency and systematic broadening of the linewidth with increasing temperature in the investigated temperature range (80–600 K). The temperature-dependence of frequency and linewidth are analysed by using anharmonic model [47, 48] (see figures S7 and S8 in supplementary material) as represented by the solid lines in figures 4(b), (d) and (f), showing the best-fit. Hence, the mode softening (and line broadening) with increasing temperature is attributed to the
Figure 5. Fano asymmetry (1/q) as a function of temperature for APd₃O₄ with A = Ca, Sr, and Sr₀.₈₅Li₀.₁₅ (a)–(c), which are compared with the 1/q values reported (d) for a few known electron–phonon coupled systems (discussed in the text). Solid lines are guide to eye.

lattice anharmonicity. Figure 5 presents the inverse of BWF asymmetry parameter (1/q) which is directly related to the strength of EPC (λₑ–ₚₗ), as a function of temperature for all the three compounds. As can be seen from figure 5(a)–(c), the coupling is almost comparable in all the three palladates, however, showing a weak temperature-dependence and differences with each other. The value of 1/q increases with increasing temperature in CaPd₃O₄, whereas it slowly decreases for SrPd₃O₄ and very clearly decreases with increasing temperature in Sr₀.₈₅Li₀.₁₅Pd₃O₄. It should be noted that the linewidth of P₁ mode in all the three compounds shows a very similar behaviour with temperature irrespective of the small differences in the temperature-dependence of asymmetry parameter (1/q). Hence, the major contribution to the linewidth comes from phonon–phonon anharmonic interactions in these systems.

In order to further understand the electronic structure and IMT along with the origin of EPC, these compounds have also been investigated using photoemission spectroscopy which will be reported elsewhere [49]. The photoemission measurements suggest that CaPd₃O₄ is slightly more insulting than SrPd₃O₄ while Sr₀.₈₅Li₀.₁₅Pd₃O₄ is metallic in nature [49]. Based on this and our Raman data we propose that there are contributions of the thermally-and also photo-excited carriers in the observed signatures of EPC. An increase in the EPC (1/q) with increasing temperature in insulating CP, as shown in figure 5(a), indicates the role of thermally excited carriers getting coupled to the phonon. On the other hand, the decreasing trend of EPC (i.e. 1/q) with temperature in SP and SLP (figures 5(b) and (c)) clearly indicate toward their excited carrier-induced metallic nature. In metallic systems, as the temperature increases the EPC decreases, as reported for LaMnO₃+δ—shown in figure 5(d) [42]. This can be attributed to an enhanced electron–electron scattering in metallic systems at high temperatures leading to reduced EPC. Further, we note that the strength of EPC (i.e. 1/q) observed in the APd₃O₄ compounds are very much comparable to the well-known systems like (a) metallic carbon nanotubes (1/q: 0.04 to 0.10 depending on the diameter) [50], LaMnO₃+δ thin films (1/q: 0.2 to 0.4 varying with temperature and oxygen partial pressure during the growth) [42], Si nanowires (1/q: 0.06 to 0.12 depending on laser power) [43], and one-layer graphene [51] etc. as shown in figure 5(d). The reasonably high EPC in narrow band-gap APd₃O₄ compounds makes them potential candidates for various possible applications in electronics, opto-electronics, and optical metamaterials.

4. Conclusions

In summary, we have synthesized polycrystalline compounds of APd₃O₄ with A = Ca, Sr, and Sr₀.₈₅Li₀.₁₅ by conventional solid-state reaction route. Four Raman active modes are observed in agreement with the group theoretical predictions. The lowest-energy optical phonon associated with palladium vibrations shows the Fano asymmetry arising from the EPC in all the three compounds. The EPC can be controlled by temperature and carrier doping in these systems. The difference in the temperature-dependence of the asymmetry parameter in these three compounds is attributed to the relative differences in their electronic structure. Interestingly, the basic ingredients required for superconductivity such as electron–electron correlation along with EPC are available in these narrow band gap semiconducting palladates. Thus, we believe that our work will motivate researchers to explore such possibility in electron/ hole doped systems.

Availability of data

The data that supports the findings of this study are available within the article [and its supplementary material].

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