First-principles study of the electronic properties of Pd$_{1-x}$Ni$_x$Te alloys

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Abstract

We have performed ab-initio electronic structure calculations to investigate the ground state properties of Pd$_{1-x}$Ni$_x$Te ($x = 0.0$–$0.20$) alloys. The PdTe and all of its alloys are paramagnetic metals. For low concentrations, the band structure remains almost unchanged and at higher concentrations, a strong redistribution of spectral weights is observed. The most striking feature of the band structure is that the bands around the Fermi energy remain almost unchanged. The calculated Fermi surfaces are remarkably robust against disorder, strongly three-dimensional and have no or negligible nesting. The density of states at Fermi energy increases monotonically with concentration ($x$). Although the contribution of Ni to the density of states at Fermi energy is increasing continuously yet, Pd and Te dominate the density of states at Fermi energy. The density of states at Fermi energy and superconducting transition temperature $T_c$ show opposite trends with respect to Ni concentration. So, density of states at Fermi level alone is not sufficient to discern the trends in $T_c$. We need to know the phonons and electron-phonon interactions as well, which at the moment are not available.

1. Introduction

Recently, PdTe a palladium-based transition metal chalcogenide has attracted the attention of experimentalists and theorists alike [1–9]. This has been partly motivated by the extensive research on iron chalcogenides [10–19], ferromagnetic instability of palladium [20, 21], exotic topological superconductivity in PdTe$_2$ [22–24] and the expectations that the study of PdTe and its alloys may shed some light on the nature of superconductivity in FeSe and related superconductors.

As an aside, PdTe$_2$ a close cousin of PdTe and member of the well known class of materials, the transition metal dichalcogenide [25, 26], has been studied rather more extensively [22–24, 27–32]. PdTe$_2$ crystallizes into a hexagonal lattice and has layered structure. It has a relatively low superconducting transition temperature $T_c \sim 1.64$ K [24] as compared to PdTe. But the interest in PdTe$_2$ is not only due to its superconductivity but it has also been shown to harbor the exotic type-II Dirac fermions [22–24].

The reports of superconductivity in PdTe date back to 1953, when it was first studied and documented by Matthias [33]. But the scientific literature on PdTe is very sparse and before the work of Karki et al [1], there were only very few reports on its physical and chemical properties [33–40]. This could have been due to the difficulties involved in synthesizing the high quality and stoichiometric samples of PdTe [37].

PdTe is a paramagnetic metal and the charge transport is dominated by electrons as confirmed by the sign of Seebeck and Hall coefficients [1, 36]. Initially, PdTe was predicted to be a strongly coupled BCS superconductor with $T_c \sim 4.5$ K [1], but later it was found to be a moderately coupled BCS type superconductor [3–6, 9]. The Pd 4d and Te 5p orbitals contribute almost equally to the density of states at the Fermi energy $N(E_F)$. Moreover, different research groups have reported different values of $N(E_F)$ lying within 1.84–2.485 states eV$^{-1}$ [1, 4, 6]. The electron-phonon coupling constant ($\lambda$) also varies from 0.648 to 1.78. The Wannier function analysis [3] of PdTe predicts strongly three-dimensional Fermi surfaces, weaker electron-electron correlations, a strong covalent character and absence of any type of magnetism [3].

Jin-Jin et al [5] have studied the effects of high pressure on electronic and thermodynamic properties of PdTe. They have found that the electronic band structure shows a strong dispersion with increasing pressure.
decrease in Ni($E_F$) and a downward shift of bands with respect to the Fermi energy is also observed. The same research group has used the density functional perturbation theory to study the phonons and electron-phonon interactions in PdTe \[6\]. They have shown that the phonon dispersion has no negative frequencies but it shows anomalous behavior around the high symmetry point \(H\). Interestingly, the entire phonon spectrum has no frequency gaps. The calculated \(\lambda\) and \(T_c\) are 0.648 and 3.2K respectively. Jianyong et al \[8\] have also studied the vibrational and superconducting properties of PdTe and their variation with high pressure. They have found that as the pressure goes from 0 to 12 GPa, \(\lambda\) goes from 0.664 to 0.529 and \(T_c\) goes from 4.2 to 2.5K, so pressure causes a monotonic decrease of \(T_c\). Increasing pressure also makes the anomaly at \(H\) less obvious, but at the same time, a similar anomaly appears around the high symmetry point \(M\).

Recently, Karki et al \[41\] have mapped out the complete phase diagram of Fe$_{1-x}$Pd$_x$Te from FeTe (for \(x = 0\)) to PdTe (for \(x = 1\)). Indeed, Fe$_{1-x}$Pd$_x$Te has a very rich phase diagram. It shows structural phase transition, magnetic ordering and exhibits metallic, non-metallic and superconducting phases. This is an ideal system to study the interplay between ferromagnetism (FM), antiferromagnetism (AFM) and superconductivity. The superconducting transition temperature decreases monotonically with increase in Fe concentration. This has been mostly attributed to the magnetic nature of iron. But it is also possible that the superconductivity in PdTe is not purely magnetic in nature of iron, but it is also possible that the superconductivity in PdTe is not purely s-wave, as speculated in \[4\]. Very recently, Reena et al \[9\] have studied the effects of Pd substitution with Ni in PdTe. The results are very interesting and demand for further investigations. They have observed that the primitive unit cell shrinks linearly with concentration (\(x\)), but the changes in lattice constants are less than \(1\%\). The \(T_c\) also decreases monotonically with \(x\) and for \(x > 0.2\) superconductivity ceases to exist. It has been suggested that Ni in PdTe and Pd$_{1-x}$Ni$_x$Te alloys is non-magnetic, which is in sharp contrast to Pd$_{1-x}$Fe$_x$Te alloys. The monotonic decrease of \(T_c\) is possibly due to the impurity scattering and change of charge carrier densities. Our main motivation to study PdTe and its alloys is to answer the questions such as (i) are Pd$_{1-x}$Ni$_x$Te alloys magnetic; (ii) whether the monotonic decrease in \(T_c\) is due to impurity scattering or there is some other mechanism behind it, and (iii) can the superconducting properties, especially the trends in \(T_c\), be understood within the framework of the BCS theory?

2. Computational details

The electronic band structure calculations are performed using the Korringa-Kohn-Rostoker Green’s function method formulated within the atomic sphere approximation \[42, 43\]. The substitution of Ni into the Pd sublattice is assumed to be purely random and treated within the single-site coherent potential approximation \[44\]. The bulk lattice constants ($a = b = 4.152\text{Å}, c = 5.672\text{Å}$) and the Wyckoff positions of \[1\] have been used to perform the self-consistent field calculations for PdTe and its alloys. We have taken the crystal structure data from \[1\], because the data is of very high quality and hence more reliable. The valence electronic configurations of Pd, Ni and Te are 4$d^9$ 5$s^2$, 3$d^8$ 4$s^2$ and 5$s^2$ 5$p^4$ respectively. The atomic sphere radii of Pd, Ni and the empty sphere E are taken to be 1.023, 1.153 and 0.733 of the average Wigner-Seitz radius (2.833 Bohr radius). The atom-atom overlap is less than \(18\%\) and the total overlap volume is \(~5\%\). The atomic sphere radii of dopant (Ni) and host (Pd) atoms are taken to be the same. Inside each atomic sphere, the partial waves are expanded up to \(\ell_{\text{max}} = 3\). For exchange-correlation potential, the generalized gradient approximation of Perdew, Burke and Ernzerhof (PBE) is used \[45\]. After each self-consistent field iteration, the core states were recalculated. For self-consistent field calculations, the Brillouin zone integration is performed using a well-converged Monkhorst-Pack \[46\] \(k\)-point grid of \(24 \times 24 \times 24\). For total energy calculations, a tight convergence threshold of \(10^{-8}\text{Ry}\) is used. The density of states (DOS) is calculated using a dense \(k\)-point grid of \(32 \times 32 \times 32\). The band structures and Fermi surfaces (FFS) are discussed, using the concept of Bloch spectral function \(A(k, E)\), it can be thought of as the \(k\)-resolved DOS. The two most commonly used settings to evaluate the Bloch spectral function (BSF) are
The Bloch spectral function $A(k, E)$ is calculated over a 2-dimensional grid formed by the wave-vector $k$ and energy $E$. This will give the band structure, along the direction specified by the wave-vector $k$.

The Bloch spectral function $A(k, E)$ is calculated over a 2-dimensional grid formed by two wave-vectors $k_1$ and $k_2$ with $E = E_F$, where $E_F$ is the Fermi energy. This will give the Fermi surface, in a plane spanned by the wave vectors $k_1$ and $k_2$.

The BSF is related to the $\mathbf{k}$-space configurationally averaged, coherent potential Green’s function $G(k, E)$ as

$$A(k, E) = -\frac{1}{\pi} \text{Im} G(k, E)$$

(1)

For a perfect crystalline solid, the Bloch spectral function consists of Dirac delta-like peaks, whereas in case of a disordered solid, these peaks generally have some finite width. These sharp peaks can cause problems during numerical integration, so a small imaginary part of 1 mRy was added to the energy for proper and efficient integration.

3. Results and discussions

3.1. Electronic structure of PdTe

The PdTe crystallizes into a NiAs type hexagonal crystal structure with space group $P6_3/mmc$ (194) and has the lattice constants $a = b = 4.152$ Å, $c = 5.672$ Å [1]. In the unit cell, Pd atom occupies 2a $(0, 0, 0)$ and Te occupies 2c $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ Wyckoff positions, figure 1 shows the primitive unit cell of PdTe.

The primitive unit cell contains a total of four atoms or two PdTe formula units. The hexagonal primitive unit cell is very similar to the tetragonal unit cell of FeTe or FeSe [10, 47, 48]. In fact, if we distort the square planes of the tetragonal unit cell along one of their diagonals then we will arrive at the hexagonal unit cell. But there are some crucial differences between the crystal structures of FeTe and PdTe. For example, FeTe is a quasi 2-dimensional material with layered structure, but PdTe is strongly 3-dimensional [3]. Transition metal (Fe) in FeTe has a tetrahedral coordination, but palladium in PdTe has an octahedral coordination [3, 8].

First we want to address the issue of magnetism in ordered PdTe. In order to rule out the possibilities of a magnetic ground state in PdTe, we have performed both the spin-polarized and spin-unpolarized calculations. We have also tried different starting magnetizations and different magnetic configurations. But within $\pm 0.1$ mRy all calculations converge to the same total energy, confirming the nonmagnetic ground state. In order to explore the possibilities of a magnetic ground state further and check its dependence on exchange-correlation functionals, we have performed the fixed spin moment (FSM) calculations using both LDA [49] and GGA [45] functionals. But, both functionals predict the nonmagnetic state to be the lowest energy state. This is consistent with the existing scientific literature [1, 3, 4].

A detailed understanding of the structure of density of states can provide a wealth of information about the electronic and magnetic properties of a material. Figures 2(a) and (b) show the sublattice and angular momentum ($\ell$) resolved DOS respectively. The calculated density of states at Fermi level $N(E_F) \sim 2.38$ states eV$^{-1}$ is lower than $1.84$
states $eV^{-1}$ [4] but very close to 2.35, 2.41 and 2.485 $eV^{-1}$ [1, 3, 6]. All other important features such as (i) The strong Pd–Te hybridization, (ii) A low DOS region just below the Fermi level, (ii) High DOS peaks and their orbital characters, (iv) A small energy gap at $\sim 2$ eV above the Fermi level etc have been reproduced very accurately. This means that ASA is well suited for the electronic properties of PdTe and its alloys.

Figure 3 shows the electronic band structure calculated along high symmetry directions in the irreducible Brillouin zone (IBZ). The band structure is plotted using the software Scilab® [50] with gray colormap representing the intensity of the Bloch spectral function $A(k, E)$. The same gray colormap is used to plot the Fermi surfaces as well. In figure 3, the electronic states or bands are well defined with zero or negligible energy width, a hallmark property of perfectly crystalline solids. It is evident from the band structure that PdTe is a metal. The overall band structure is in excellent agreement with the previous theoretical studies [1, 3, 6, 8, 51].

The Fermi surface is a constant energy surface ($E = E_F$) in reciprocal space which separates the occupied and unoccupied states. A detailed knowledge of the Fermi surface is crucial to determine the effective dimensionality and the effects of Fermi surface nesting. Figures 4(a) and (b) show the Fermi surfaces in $\Gamma - M - L - \Delta$ and $\Gamma - K - H - \Delta$ planes respectively. We can compare these 2-dimensional Fermi surfaces with the 3-dimensional Fermi surfaces [51], but to do that, first we have to take the 2-dimensional cuts of 3-dimensional Fermi surfaces corresponding to the four bands that cross the Fermi energy [51], and then assemble the results into the first Brillouin zone. This process is very cumbersome and prone to errors. Instead, we will compare the Fermi surfaces with band structure and look for the inconsistencies (if any). From figures 4(a) and (b), the high symmetry directions $\Gamma - \Delta$, $\Gamma - M$ and $\Gamma - K$ have three, one and three Fermi surfaces respectively, which is consistent with figure 3. It is worth noting that degeneracy in band structure can reduce the number of Fermi surfaces. In summary, the atomic sphere approximation is an excellent choice to study the electronic and magnetic properties of PdTe and its alloys.
Figure 5 shows the variation of the Fermi surfaces in $\Gamma - M - K$ plane with respect to $k_z$, where $k_z$ is given in the units of $\frac{2\pi}{a}$. The first and last surface plots in figure 5 correspond to the Fermi surfaces in $\Gamma - M - K$ ($k_z = 0$) and $A - L - H$ ($k_z = \frac{a}{2}$) planes respectively. It is very clear that the Fermi surfaces show a strong variation with respect to $k_z$, confirming the 3-dimensional nature of Fermi surfaces. It also rules out the possibilities of Fermi surface nesting in PdTe.

### 3.2. Electronic structure of Pd$_{1-x}$Ni$_x$Te alloys

The effects of doping are strongly tied with the material’s chemistry and the crystal structure. For example, missing atoms or vacancies in a solid lead to the formation of dangling bonds with unshared electrons. Under
appropriate conditions, the electron spins at these vacant sites can order preferentially to give rise to a magnetic ground state [52–55]. Doping can add charge carriers to the system, alter the electron-phonon interactions and influence the electronic band structure of the material.

In order to check the propensity of Pd$_{1-x}$Ni$_x$Te alloys towards magnetism, we have performed both the spin-polarized and spin-unpolarized calculations for all values of ($x = 0.01–0.20$). We have even tried (i) different starting magnetizations (to break the spin symmetry), (ii) different magnetic configurations (by using different magnetic moments for different sites), (iii) fixed spin moment method (which usually does not suffer from the convergence issues) and (iv) different exchange-correlation functionals (both LDA and GGA). The total magnetic moments are either zero or less than 0.01 $\mu_B$, and within $\pm 0.1$ mRy, all calculations converge to the same total energy. It means that PdTe and all of its Pd$_{1-x}$Ni$_x$Te alloys (for $x = 0.01–0.20$) are non-magnetic.

This is consistent with the experimental results [9]. It is worth mentioning that the Fe doping in PdTe leads to a very rich phase diagram where ferromagnetism coexists with short-range antiferromagnetism and superconductivity [41]. We will discuss the results of spin-unpolarized calculations only.

As mentioned in previous discussion, a low DOS region lies just below the Fermi level. So, if we dope PdTe with extra holes and assume a rigid band behavior, then it will lead to a reduced DOS at Fermi level, simply because the Fermi level has moved to the low DOS region. So, hole doping may not be an effective way to

![Figure 6](image_url)
enhance $T_c$ in these alloys. Also, the DOS above the Fermi level remains relatively flat for almost 1 eV, so even the electron doping may not be helpful. Nonetheless, doping a magnetic element such as Fe, Co or Ni in PdTe may provide answers to the questions, like why Ni doping is non-magnetic but Fe doping is not or do the magnetism and superconductivity really coexist? Nickel (Ni$^{2+}$) is isovalent to palladium (Pd$^{2+}$), so the substitution of Pd with Ni should neither add nor remove the carriers at the Fermi level. Figure 6 shows the calculated DOS for Pd$_{1−x}$Ni$_x$Te alloys. For $x = 0.01$, the DOS is almost unchanged consistent with the fact that $T_c$ is nearly unchanged for Pd$_{0.99}$Ni$_{0.01}$Te [9]. For $x > 0.01$, the density of states show a very strong redistribution of spectral weights with increasing Ni concentration ($x$). On the other hand, density of states above the Fermi level remains almost unchanged, apart from the broad peak at $\sim$4eV which gets suppressed with increasing concentration ($x$). For low concentrations ($x < 0.07$), the density of states at Fermi level $N(E_F)$ is still dominated by Pd ($d$) and Te ($p$) states, but for high concentrations ($x > 0.07$), Ni ($d$) states also contribute significantly to $N(E_F)$. The high DOS peaks at $\sim 3.0$ eV and $\sim 2.3$ eV below the Fermi level decrease continuously as $x$ increases. Since these peaks are mainly composed of Pd states, so the contribution of Pd decreases as $x$ increases. The low DOS region just below the Fermi level becomes less and less obvious with increasing $x$. A new peak starts appearing at $\sim 1.25$ eV, which is mainly composed of Ni ($d$) states and increases monotonically with increasing concentration ($x$). In general, peaks with Pd contribution in them are losing their spectral weights with increasing $x$, which is mostly getting transferred to the new peak at $\sim 1.25$ eV. The contribution of Te remains almost constant (as if it does not care whether it has to form bonds with Pd or Ni). The very low energy states ($E < 10$ eV) are not shown, because they do not participate in chemical bonding and have little or no effect on the electronic properties of materials (apart from the indirect effects coming from their hybridization with valence states). The disorder induced effects such as broadening and smoothing of sharp peaks are present almost everywhere.

Figure 7 shows the variation of total and sublattice projected $N(E_F)$ with dopant concentration ($x$). It is clear from figure 7 that the total $N(E_F)$ increases monotonically from 2.38 states eV$^{-1}$ (for $x = 0.0$) to 2.61 states eV$^{-1}$ (for $x = 0.2$). The individual contribution from Pd and Te to $N(E_F)$ decreases monotonically with increasing $x$. Maybe, because Pd is getting removed from the system as more and more Ni is added in. The contribution from empty spheres to $N(E_F)$ is almost constant and it is very small. Although, the contribution of Ni to $N(E_F)$ is increasing continuously yet Pd and Te dominate the $N(E_F)$. The total density of states at Fermi level $N(E_F)$ and $T_c$ show opposite trends with respect to Ni concentration ($x$). In other words, $T_c$ decreases with increasing concentration ($x$) [9]. Similar trends have been observed for Pd$_{1−x}$Fe$_x$Te alloys as well, but these alloys are magnetic and decrease in $T_c$ can be attributed to the pair-breaking effects of magnetism [7]. But Pd$_{1−x}$Ni$_x$Te alloys are non-magnetic, so it cannot be magnetism. Further work is needed to reconcile these contradictory results.

![Figure 7. The total and sublattice projected density of states of Pd$_{1−x}$Ni$_x$Te alloys at the Fermi energy.](image-url)
The calculated band structures of Pd$_{1-x}$Ni$_x$Te alloys are shown in figure 8. The electronic band structure results reinforce the observations made on the basis of DOS. For $x = 0.01$, the band structure remains almost unchanged. As we increase the concentration ($x$) further, the bands in the energy range $\sim -6.0$ to $-1.0$ eV start getting diffused, consistent with the strong redistribution of spectral weight observed in DOS. Except $\Gamma - H$ direction, all other high symmetry directions have at least one band crossing the Fermi level. This confirms that PdTe and all of its alloys are metallic in nature [9]. The most striking feature of the band structure is that the bands around the Fermi level (including the Dirac cones like feature along $M - L$ direction) remain almost unchanged.

Figures 9 and 10 show the calculated Fermi surfaces of Pd$_{1-x}$Ni$_x$Te alloys in $\Gamma - M - L - A$ and $\Gamma - K - H - A$ planes respectively. The Fermi surfaces are impervious to the increasing disorder and have no or negligible width, even their shapes are preserved. It is hard to see, but the Fermi surfaces around the high symmetry point A and $\Gamma$ are expanding with concentration ($x$) but very slowly. These effects are much more evident for higher values of ($x > 0.30$).

The number of Fermi surfaces (or equivalently the number of bands crossing the Fermi level) along each high symmetry direction are also unchanged.
4. Conclusions

We have explored the ground state properties of Pd$_{1-x}$Ni$_x$Te ($x = 0.0–0.20$) alloys using state-of-the-art KKR-ASA–CPA method. The convergence of total energy with respect to all relevant computational parameters was carefully checked. We have also demonstrated that the atomic sphere approximation is as accurate as the pseudo-potential methods and an excellent choice to study the electronic structure of PdTe and its alloys. All Pd$_{1-x}$Ni$_x$Te alloys are nonmagnetic. For low concentrations, the band structure remains almost unchanged. But at higher concentrations, the bands start getting diffused along with a strong redistribution of spectral weights. The most striking feature of the band structure is that the bands around the Fermi level remain almost unchanged. The Fermi surfaces are remarkably robust against disorder, strongly three dimensional and has no or negligible nesting.
The total $N(E_F)$ increases monotonically with concentration ($x$). The individual contribution from Pd and Te to $N(E_F)$ decreases monotonically with increasing $x$. Maybe, because Pd is getting removed from the system as more and more Ni is added in. Although, the contribution of Ni to $N(E_F)$ is increasing continuously yet Pd and Te dominate the $N(E_F)$. The total density of states at Fermi level $N(E_F)$ and $T_c$ show the opposite trends with respect to Ni concentration ($x$). In other words, $T_c$ decreases with increasing concentration ($x$) [9]. Similar trends have been observed for $\text{Pd}_{1-x}\text{Fe}_x\text{Te}$ alloys as well, but these alloys are magnetic and decrease in $T_c$ can be attributed to the pair-breaking effects of magnetism [7, 41]. But $\text{Pd}_{1-x}\text{Ni}_x\text{Te}$ alloys are nonmagnetic, so it cannot be magnetism. Transition metal (Ni) doping in FeSe or FeSe$_{1-x}$Te also reduces $T_c$ and leads to the metal–to–insulator transition [56–58]. The density of states at Fermi level alone is not sufficient to discern the trends in $T_c$. We need to know the phonons and electron-phonon interactions as well, which at the moment are not available. In this work, we have investigated the electronic and magnetic properties of $\text{Pd}_{1-x}\text{Ni}_x\text{Te}$ ($x = 0.0$–0.20) alloys. But, for a complete understanding of the superconducting pairing mechanism and pairing symmetry, we have to understand both the normal and the superconducting states in great details. This is why, we should also study the electronic and magnetic properties of $\text{Pd}_{1-x}\text{Ni}_x\text{Te}$ alloys ($x > 0.30$). In order to further clarify the role of Ni and explain the opposite trends in $T_c$ and $N(E_F)$, additional theoretical work is required. We hope that our theoretical work will encourage experimentalists to further investigate the electronic structure of these alloys, using sophisticated tools such as the angle-resolved photoemission spectroscopy so that a detailed comparison with theory can be made.

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