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Electronic structure and superconductivity in Pd-Ag-H and Pd-Rh-H alloys

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Using the augmented-plane-wave method we have calculated the energy bands and the densities of states (DOS) of RhH, PdH, and AgH. We have also calculated the DOS for the nonstoichiometric hydrides $Pd_{1-y}Ag_yH_x$ and $Pd_{1-y}Rh_yH_x$ within the virtual-crystal approximation (VCA) and the rigid-band approximation (RBA). We present evidence from coherent-potential-approximation calculations that our DOS values in the vicinity of the Fermi level are reliable. The DOS decomposed per site and angular-momentum component are used to calculate the electron-phonon interaction and the superconducting transition temperature, T_c, for various compositions of the above alloys. Our results are in good agreement with experiment and provide a satisfactory understanding of the variation of T_c with x and y and also of the isotope effect in these systems.

I. INTRODUCTION

In a series of recent papers[1–6] we have presented a theoretical interpretation of the phenomenon of superconductivity in the palladium-hydrogen system. This theory is based on elaborate band-structure calculations, neutron scattering data and an application to compounds[7] of the McMillan[8] and Gaspari-Gyorffy[9] theories of the electron-phonon interaction. Our results show that the high value of the superconducting transition temperature T_c in PdH (PdD) is mainly due to the soft-optic-mode phonon frequencies which are associated with local hydrogen vibrations. This is a quantitative verification of an earlier suggestion by Ganguly.[10] Ganguly[10] also proposed that the observed isotope effect is caused by the effective increase of the Pd-H force constant over the Pd-D force constant, due to enhanced anharmonicity of the H motion. Using our band-structure results[4] and neutron scattering data[11,12] for both PdD and PdH, we have again confirmed quantitatively Ganguly's idea. We have also calculated the x dependence of T_c for PdH_x and PdD_x. In this calculation[3,4] we employed first the rigid-band approximation (RBA), which allowed us to use the band structure of the stoichiometric case ($x = 1.0$). We then confirmed the validity of the RBA, for a narrow energy range around the Fermi level, E_F by performing coherent-potential-approximation (CPA) calculations.[5] The physical picture which emerged from both the RBA and the CPA approaches is that T_c increases with x, because the wave functions at E_F become more hydrogen s-like in character. This is manifested by the increasing with x value of the hydrogen-site s-like density of states at E_F. This means that the electrons at E_F have high probability of being found around the H (D) sites and consequently they couple effectively with the relatively soft H (D) "local" mode.

We now present similar calculations of the superconducting properties of $Pd_{1-y}Ag_yH_x$ and $Pd_{1-y}Rh_yH_x$. These calculations were performed by the augmented-plane-wave (APW) method and employed the virtual-crystal approximation (VCA) to simulate the substitution of Pd by Ag or Rh, and the rigid-band approximation (RBA) to describe the vacancy disorder of the hydrogen sublattice. In one of our calculations we removed the RBA by applying the CPA on the hydrogen site but still retaining the VCA on the metal site.

A preliminary account of the present results was given in Ref. 6.

II. METHODS OF CALCULATION

The calculations were done by the (APW) method in the NaCl structure and with the lattice constant of

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$PdH_{1.0}$. ($a_0 = 4.09$ Å).[13] According to the measurements of Axelrod and Makrides[14] and Becker,[15] and recent calculations by Williams *et al.*[16] we should expect that the maximum variation in the lattice spacing is no more than 2% as y varies. In fact we have repeated our $Pd_{0.5}Ag_{0.5}H$ calculations with a lattice constant 2% greater than that of PdH and the resulting densities of states (DOS) at E_F were changed by only 7%, which does not change the conclusions of the present work. We generated potentials for the alloys in the (VCA) by averaging the $PdH_{1.0}$ with the $AgH_{1.0}$ and the $RhH_{1.0}$ potentials. Because of the uncertainty in the lattice constant and the VCA assumption we did not find it meaningful to carry these calculations to self-consistency. The calculations were performed by the spin-independent relativistic APW method first proposed by Mattheiss[17] and recently improved by Koelling and Harmon.[18] The exchange potentials were determined using the $X\alpha$ parameters of Schwarz.[19] The APW calculations were done on a mesh of 89 k points in the $\frac{1}{48}$th of the Brillouin zone. The energy eigenvalues and the electronic charges inside the muffin-tin spheres were interpolated using a variant of the QUAD method,[20] which produces the DOS decomposed per site and angular-momentum component. The total DOS, n_t of $PdH_{1.0}$, $AgH_{1.0}$, $RhH_{1.0}$, and $Pd_{0.7}\,Ag_{0.3}\,H_{1.0}$ and their s-like hydrogen components, $n_{s\,H}$, are shown in Fig. 1. The similarity of the $PdH_{1.0}$, $AgH_{1.0}$, and $RhH_{1.0}$ DOS suggest that the VCA is probably adequate.

In order to clarify the validity of the VCA for the present system we have calculated the ratio $R = \Delta / W_d$, where

$$\Delta = \Delta_{sd}^{\mathrm{PdH}} - \Delta_{sd}^{\mathrm{AgH}} ,$$

with $\Delta_{sd} = E(\Gamma_{25}') - E(\Gamma_1)$ being the separation between the d bands and the hydrogen bonding states, and

$$W_d = \tfrac{1}{2}[(X_5 - X_3)_{\mathrm{PdH}} + (X_5 - X_3)_{\mathrm{AgH}}]$$

being the average d bandwidth of PdH and AgH. We have found $R = 0.37$ which is not small enough to completely justify the VCA.[21,22] However in viewing the DOS figures of Stocks *et al.*[22] for the Pd-Ag alloys we note that a separation of the d bands occurs only for the high Ag concentrations. This suggests that in the Pd-rich range our use of the VCA is a rea-

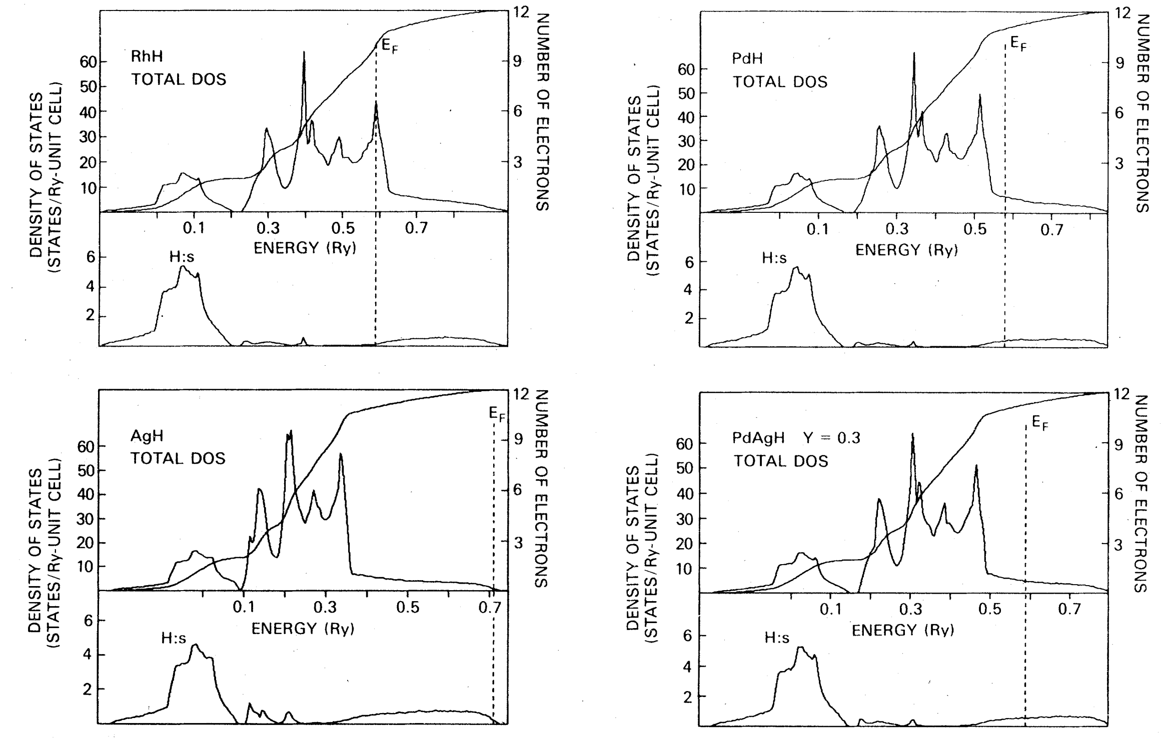

FIG. 1. Total and s-like hydrogen densities of states for RhH, PdH, AgH, and $Pd_{0.7}Ag_{0.3}H$. The energy scale is given with respect to the respective muffin-tin zero for each compound.

TABLE I. T_c, $\omega_{\log}$, η, and λ as a function of hydrogen concentration x for $Pd_{0.85}Ag_{0.15}H_x$ and $Pd_{0.85}Ag_{0.15}D_x$. η is expressed in units of eV/Å^2 and $\omega_{\log}$, T_c in °K.

x	η_H	η_{Met}	λ_H	λ_D	λ_{Met}	$\omega_{\log}$ (H)	$\omega_{\log}$ (D)	T_c (H)	T_c (D)
1.0	0.63	0.88	0.60	0.73	0.19	552.3	388.2	20.2[a]	19.8[a]
0.94	0.56	0.84	0.53	0.65	0.18	541.1	382.9	15.3[a]	15.8[a]
0.91	0.53	0.84	0.50	0.61	0.18	531.0	377.9	13.0	13.8
0.78	0.40	0.83	0.38	0.46	0.18	488.3	356.9	5.8	7.1

[a] These high values of T_c cannot be realized probably due to resistance of the system to absorb hydrogen in amounts corresponding to $x \geqslant 0.94$ (see Refs. 15 and 27).

sonable approximation. Further evidence that the VCA is reliable for the Pd-rich alloys can be found in the recent work of Temmerman *et al.*[23] These authors have applied the muffin-tin CPA in the Cu-Ni system and they have concluded that for the Ni-rich alloys the energy bands are for the most part like smeared out virtual-crystal bands.

Figure 1 also implies that the RBA can be used here in the same manner as it was applied in our Pd-H work.[4] Studying the figure within the RBA we note that n_t decreases as we move from the 10 to the 12 electron mark, while $n_{s\,H}$ increases in the range from the 10 to approximately the 11.75 electron mark. Note that the number of electrons per unit cell equals to $10 \mp y + x$; where the (−) sign corresponds to Rh and the (+) sign to Ag.

To obtain the electron-phonon interaction η we have applied the theory of Gaspari and Gyorffy,[9] which utilizes the total and decomposed DOS, and the scattering phase shifts all evaluated at E_F. It was shown previously[7] that due to the large mass difference between Pd and H, one can decouple η into a term η_H which corresponds to optic-mode scattering and a term $\eta_{PdAg,Rh}$ which corresponds to scattering from the acoustic modes.

We have found that the important quantity which determines the T_c variation in these systems is η_H. As is shown in Tables I–III, $\eta_{Pd,Ag}$ is nearly constant in the hydrogen-rich region where superconductivity occurs, and when divided by $M\langle\omega^2\rangle$ gives a much smaller contribution to the total λ than that given by η_H. The quantity η_H is dominated by the first term of the Gaspari-Gyorffy formula, i.e.,

$$\eta_H \approx \frac{E_F}{\pi^2 n_t}\,\frac{2 n_{s\,H} n_{p\,H}}{n_{s\,H}^{(1)} n_{p\,H}^{(1)}}\sin^2(\delta_{p\,H}-\delta_{s\,H})\,, \tag{1}$$

where E_F is the Fermi energy with respect to the muffin-tin zero, n_t the total DOS at E_F, $n_{s\,H}$ and $n_{p\,H}$ the hydrogen-site s- and p-like DOS at E_F, $n_{s\,H}^{(1)}$ and $n_{p\,H}^{(1)}$ the "free-scatterer" DOS as defined by Gaspari and Gyorffy, and $\delta_{s\,H}$ and $\delta_{p\,H}$ the scattering phase shifts evaluated at E_F and at the muffin-tin radius R_s.

In order to calculate T_c, in our McMillan-like approach, we need to know the coupling constant,

$$\lambda = \frac{\eta_H}{M_H\bar{\omega}_H^2} + \frac{\eta_{Met}}{M_{Met}\bar{\omega}_{Met}^2}\,, \tag{2}$$

where

$$\bar{\omega}_s^2 = \langle\omega\rangle_s / \langle\omega^{-1}\rangle_s$$

and

$$\langle\omega^m\rangle_s = \int_0^\infty \omega^m F_s(\omega)\,d\omega$$

and the subscript Met stands for metal with $F_s(\omega)$ the site-decomposed phonon DOS. As we have discussed in our PdH work[4] we obtain η_H and η_{Met} from our band-structure results while we determine the denominators in Eq. (2) from the measured phonon DOS.[11,12] However, except for the PdH (PdD) data, the only data we have found on the phonon spectra are the neutron scattering measurements of Chowdhury and Ross[24] for $Pd_{1-y}Ag_yH_x$ with $y \approx 0.2$. These data show that alloying PdH with small amounts of Ag does not alter the optic-mode frequency significantly. It seems therefore reasonable, for at least small Ag or Rh concentrations, to proceed with our calculations using the PdH and PdD values of $\langle\omega^m\rangle_H$ and to scale $\langle\omega^m\rangle_{Met}$ of PdH using the Debye temperatures of Pd, Ag, and Rh. As in our PdH work[3,4] we have used the following relationship

$$M_H\bar{\omega}_H^2 = 1.2 M_D\bar{\omega}_D^2 \tag{3}$$

to account for anharmonicity of the hydrogen motion.[12] We have used the following equation for T_c, due to Allen and Dynes.[25]

$$T_c = f_1 f_2 \frac{\omega_{\log}}{1.2}\exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right], \tag{4}$$

with $f_1 = f_2 = 1$, and

$$\omega_{\log} = 2\langle\omega\rangle - \langle\omega^2\rangle^{1/2}\,,$$

TABLE II. T_c, $\omega_{\log}$, η, and λ as a function of hydrogen concentration x for $Pd_{0.7}Ag_{0.3}H_x$ ($Pd_{0.7}Ag_{0.3}D_x$). η is expressed in units of eV/Å^2 and $\omega_{\log}$, T_c in °K.

x	η_H	η_{Met}	λ_H	λ_D	λ_{Met}	$\omega_{\log}$ (H)	$\omega_{\log}$ (D)	T_c (H)	T_c (D)
1.0	0.80	0.76	0.76	0.92	0.17	596.0	408.6	31.0[a]	28.3[a]
0.9	0.65	0.78	0.61	0.75	0.18	564.7	393.7	20.8[a]	20.3[a]
0.86	0.57	0.78	0.54	0.66	0.18	545.5	384.4	15.4	15.9
0.8	0.48	0.78	0.45	0.55	0.18	518.6	371.3	9.9	11.1
0.7	0.34	0.74	0.32	0.39	0.17	469.0	346.5	3.0	4.2
0.6	0.24	0.74	0.23	0.28	0.17	405.7	313.9	0.7	1.2

[a] These high values of T_c cannot be realized probably due to resistance of the system to absorb hydrogen in amounts corresponding to $x \geqslant 0.94$ (see Refs. 15 and 27).

with

$$\langle\omega\rangle = \frac{2(\alpha_H^2 + \alpha_{Met}^2)}{\lambda},$$

$$\langle\omega^2\rangle^{1/2} = \frac{2(\alpha_H^2\langle\omega\rangle_H + \alpha_{Met}^2\langle\omega\rangle_{Met})^{1/2}}{\lambda},$$

$$\alpha_H^2 = \frac{\eta_H}{2M_H\langle\omega\rangle_H}, \quad \alpha_{Met}^2 = \frac{\eta_{Met}}{2M_{Met}\langle\omega\rangle_{Met}}.$$

We have used here $\mu^* = 0.13$ and not values derived using the Bennemann-Garland formula[26] as we did previously.[4] The reason is that our values of $\eta_{H(D)}$ from the non-self-consistent calculations of PdH — which are approximately 10% higher than those found by the self-consistent calculation[4] — fit better the measured T_c's if we use $\mu^* = 0.13$. We believe that this change is appropriate since our alloy calculations were not performed self-consistently.

III. RESULTS AND DISCUSSION

Our results, for the superconducting properties of these alloys, are shown in Tables I–IV and also in Figs. 2–4. Figure 2 shows η_H versus hydrogen concentration x for RhH_x, PdH_x, AgH_x, $Pd_{0.5}Rh_{0.5}H_x$, $Pd_{0.9}Rh_{0.1}H_x$, $Pd_{0.85}Ag_{0.15}H_x$, $Pd_{0.7}Ag_{0.3}H_x$, and $Pd_{0.5}Ag_{0.5}H_x$. We note from this figure that (i) addition of Rh decreases η_H, (ii) addition of Ag increases η_H, (iii) for a given Pd to Rh (Ag) ratio, the addition of more H increases η_H, and (iv) for the case of AgH_x, η_H drops sharply as we approach $x = 1$. We have studied Eq. (1) and found that the increase of η_H is almost entirely determined by an increase of the DOS ratio $n_{s\,H}/n_t$, with the other quantities varying very slowly with x. These observations were exploited in our CPA calculations[5] for PdH_x where we

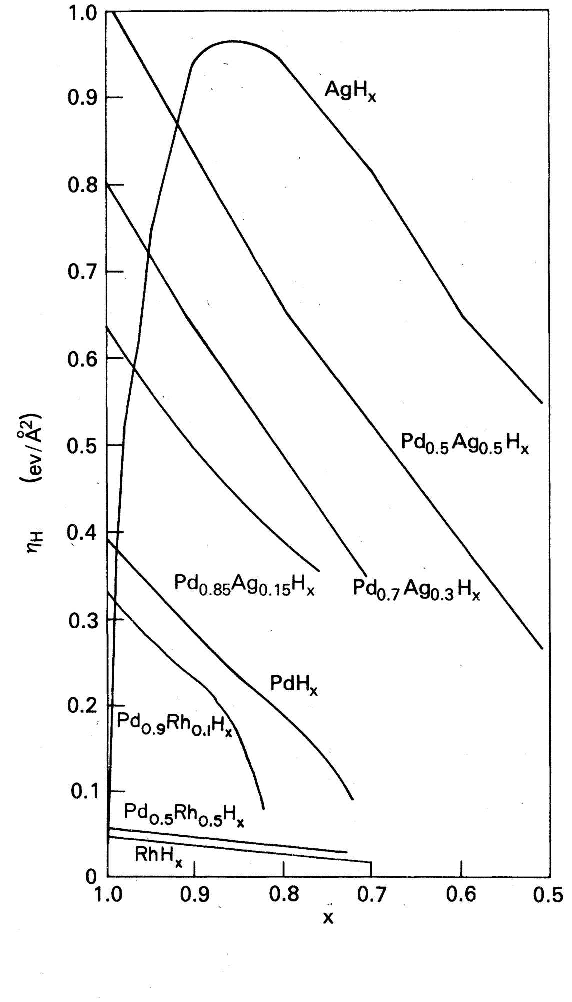

FIG. 2. Hydrogen-site electron-phonon interaction η_H plotted as a function of hydrogen concentration x.

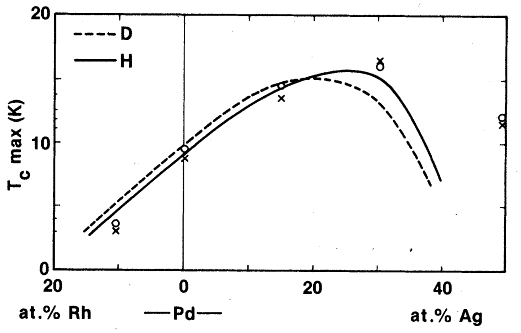

FIG. 3. Measured values of T_c (after Stritzker) plotted vs y for the optimum value of x which gives the maximum T_c. Our calculated values indicated by ○ and × for the deuteride and hydride respectively, correspond, from left to right, to the following values of x: 1.0, 1.0, 0.9, 0.85, and 0.70.

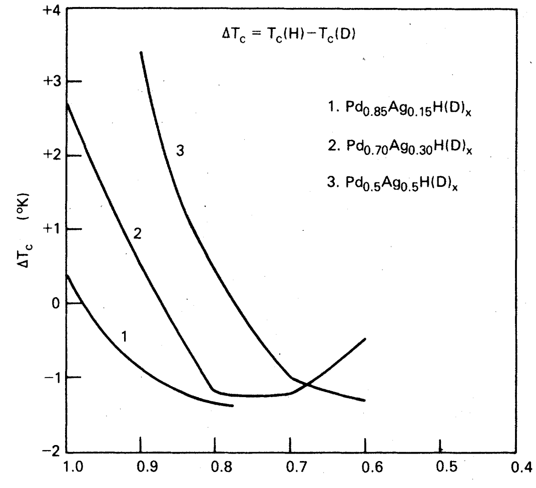

FIG. 4. ΔT_c plotted as a function of hydrogen concentration x. $\Delta T_c > 0$ denotes normal isotope effect and $\Delta T_c < 0$ denotes inverse isotope effect.

employed the approximate formulas

$$\eta_H \approx \frac{n_{s\,H}}{n_t}(E_F)\ , \quad \eta_{Pd} \approx \frac{n_{dPd}}{n_t}(E_F)\ , \tag{5}$$

where the proportionality constants C_H and C_{Pd} were determined from the APW results at $x = 1.0$.

We have applied this CPA approach in our present work only for $Pd_{0.5}Ag_{0.5}H_x$. The results, shown in parenthesis in Table III, are in reasonable agreement with the VCA-RBA results. We remind the reader that the CPA theory was applied only on the hydrogen-site sublattice and the Pd-Ag substitutional disorder was still treated within the VCA.

From Tables I–IV, we note that for a given H (D) concentration x, T_c decreases monotonically with additions of Rh and increases monotonically with additions of Ag in agreement with experiment[27] (see Fig. 3). Also for a given Ag or Rh concentration, T_c increases monotonically with the addition of H or D. Our calculated values, shown in Tables I–IV, are in good agreement with experiment[27] for those alloy compositions for which measurements exist. Our unusually high values for T_c predicted for large hydrogen concentration cannot be achieved experimentally because, according to Stritzker[28] and Becker,[15] it appears that the addition of Ag decreases the amount of H (D) which can be absorbed by the system. Note in this connection that pure AgH cannot form because hydrogen cannot be absorbed by Ag.

As is also shown in Tables I–IV, our results show that the inverse isotope effect becomes normal with the addition of Ag, again in agreement with experi-

TABLE III. T_c, $\omega_{\log}$, η, and λ as a function of hydrogen concentration x for $Pd_{0.5}Ag_{0.5}H_x(Pd_{0.5}Ag_{0.5}D_x)$. η is expressed in units of eV/Å^2 and $\omega_{\log}$, T_c in °K.

x	η_H	η_{Met}	λ_H	λ_D	λ_{Met}	$\omega_{\log}$ (H)	$\omega_{\log}$ (D)	T_c (H)	T_c (D)
1.0	1.05	0.69	0.99	1.21	0.17	628.6	423.5	47.5[b]	40.0[b]
0.9	0.84(0.89)[a]	0.68(0.81)[a]	0.79(0.84)[a]	0.97	0.16(0.19)[a]	605.3	412.5	33.5[b]	30.1[b]
0.8	0.66(0.77)[a]	0.69(0.90)[a]	0.62(0.73)[a]	0.76	0.17(0.21)[a]	572.3	396.8	21.1[b]	20.6[b]
0.75	0.58	0.70	0.55	0.67	0.17	551.7	386.8	15.8[b]	16.2[b]
0.7	0.51(0.61)[a]	0.70(1.0)[a]	0.48(0.58)[a]	0.59	0.17(0.24)[a]	532.0	377.2	11.4	12.4
0.6	0.39	0.73	0.37	0.45	0.18	480.3	351.4	5.3	6.6

[a] CPA results.

[b] These high values of T_c cannot be realized probably due to resistance of the system to absorb hydrogen with $x > 0.7$; and also because of a possible change of the optic-mode phonon frequencies.

TABLE IV. T_c, $\omega_{\log}$, η, and λ as a function of hydrogen concentration x for $\mathrm{Pd_{0.9}Rh_{0.1}H}_x(\mathrm{Pd_{0.9}Rh_{0.1}D}_x)$. η is expressed in units of eV/Å^2 and $\omega_{\log}$, T_c in °K.

x	η_{H}	η_{Met}	λ_{H}	λ_{D}	λ_{Met}	$\omega_{\log}$ (H)	$\omega_{\log}$ (D)	T_c (H)	T_c (D)
1.0	0.33	0.84	0.31	0.38	0.15	493.3	361.9	2.3	3.4
0.92	0.24	0.86	0.23	0.28	0.15	436.5	333.8	0.5	1.0
0.84	0.11	0.84	0.11	0.13	0.15	312.4	268.4	0.0	0.0

ment.[27] This is also demonstrated in Fig. 4 where we have plotted ΔT_c as a function of x. An inspection of Eq. (4) and of Tables I–IV reveals that isotopic differences in T_c result from differences in the values of $\omega_{\log}$ and λ. We note that the ratio, $\omega_{\log}$ (H)/$\omega_{\log}$ (D), is not very sensitive to x and y, remaining at ~ 1.4. Also, from Eq. (3) regarding the anharmonicity of the hydrogen (deuterium) motion we have $\lambda_{\mathrm{D}} = 1.2\lambda_{\mathrm{H}}$ for all x and y. Thus the key to understanding the x and y dependence of the isotope effect is in the behavior of the exponential factor as a function of λ. For those λ for which $\lambda_{\mathrm{H}} \lesssim 0.57$, the exponential factor is a sufficiently strong function of λ to reverse the normal isotope effect. For $\lambda_{\mathrm{H}} \gtrsim 0.55$ the $\omega_{\log}$ prefactor wins over the exponential factor and we have $T_c(\mathrm{H}) > T_c(\mathrm{D})$ as in a normal isotope effect.

It must be stressed that the various assumptions and approximations made are well justified only within a restricted region in the x-y plane. The assumption of a NaCl structure with the Ag (or Rh) substituting randomly for Pd is probably valid up to a maximum value of y beyond which lattice instabilities seem to take place[10]; the validity of the assumption that $\langle\omega^2\rangle_{\mathrm{opt}}$ does not change appreciably with y restricts even more the values of y to $y \lesssim 0.3$. The value of x has an upper bound $x_c(y)$, close to $1-y$, beyond which the hydrogen is totally lost.[15,28] According to our analysis in Refs. 4 and 5 the RBA is valid for $x \gtrsim 0.7$. Finally due to the relative small value of the parameter R, discussed in Sec. II, the VCA is not expected to introduce significant errors. Hence, we believe our results are reliable for $0.7 \lesssim x \lesssim x_c(y)$ and $0 \leqslant y \leqslant 0.3$ with some uncertainty in the precise value of the limits. Within this range the agreement with the experimental data is very good. It should be mentioned that no adjustable parameters, other than setting $\mu^* = 0.13$, were used in our calculations.

We think that the present work provides a good understanding of the variation of T_c in Pd-based hydrides. It shows that this variation is mainly controlled by the hydrogen s-component of the eigenstates at the Fermi level. We believe that outside the x,y range stated above, structural instabilities or possibly stiffening of the hydrogen optic mode prevent further increase in T_c.

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