Prediction of high-temperature superconductivity in hexagonal and rhombohedral phases of metallic hydrogen

T. W. Barbee III and Marvin L. Cohen
Department of Physics, University of California, Berkeley, Berkeley, California 94720
and Materials and Chemical Sciences Division,
Lawrence Berkeley Laboratory, Berkeley, Berkeley, California 94720
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Under extreme pressure, hydrogen is predicted to transform from a low-pressure molecular solid into an atomic solid. Several candidate structures for the atomic solid are studied as candidates for superconductivity. In particular, the $9R$ (α–Sm) structure is found to be stable with a predicted transition temperature T_c = 140–170 K. Results for hexagonal phases are also discussed.

I. INTRODUCTION

At low pressures and temperatures, hydrogen occurs in an insulating molecular phase. Over 50 years ago it was predicted[1] that the application of extreme pressure could break the molecular bond and cause hydrogen to form a monatomic solid that would then be metallic. Many theorists[1–5] have attempted to predict the metallization pressure of hydrogen. Early efforts[1] focused on the molecular-to-atomic transition, but more recent work[2–5] predicts that metallization should occur via band overlap within the molecular phase at a pressure of 1.5 – 2.5 Mbar. Under still higher pressure, the molecular bond will break and hydrogen is predicted[3–5] to transform into an atomic metal. This transition is estimated to occur at pressures in the neighborhood of 4 Mbar, with further transitions between atomic phases possible at even higher pressures.

It was also predicted[6,7] that metallic hydrogen could be a superconductor in the atomic phase, but predictions[7–10] of the transition temperature varied widely. *Ab initio* total-energy calculations[5] predict that a simple hexagonal phase of hydrogen is particularly stable relative to the cubic phases most often considered[3,8–11] previously. Recently, we predicted[12] that hydrogen in a distorted simple hexagonal structure would have a high transition temperature. In this paper, we present further results for this structure and also for the simple hexagonal structure and for the $9R$ (α-Sm) structure.

Our previous total-energy study[5] of hydrogen predicted that the molecular-to-atomic transition should occur at a pressure slightly below 4 Mbar, and that hydrogen should assume an anisotropic simple hexagonal (sh) structure with a c/a ratio of 0.6 at a density corresponding to a Wigner-Seitz radius r_s = 1.3 atomic units. The charge density for hydrogen in the sh structure is shown in Fig. 1. The electrons are concentrated in filaments along the hexagonal axis, and the bonding is anisotropic and covalent. It was previously noted[13] that such bonding is favorable for the occurrence of superconductivity; therefore, we studied the superconducting properties of atomic metallic hydrogen.

In Sec. II, we present the formalism within the framework of standard BCS-Eliashberg[14,15] theory for our calculations of the electron-phonon coupling λ and the superconducting transition temperature T_c. The results for several candidate structures suggested by total-energy studies are then presented and discussed, beginning with the simple hexagonal (sh) and distorted simple hexagonal (dsh) structures. These are found to be unstable, so we have considered a third structure, namely, the $9R$ (α-Sm), which our calculations predict to be stable. The

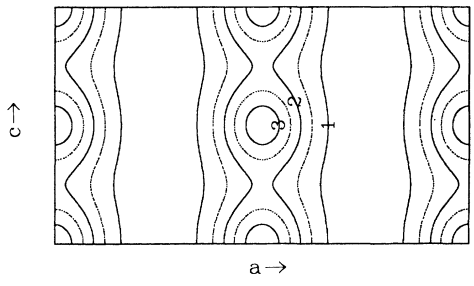

FIG. 1. Charge density $\rho(\mathbf{r})$ for hydrogen in the simple hexagonal structure discussed in the text in a plane containing the hexagonal axis c. The electrons are concentrated in filamentary structures along the hexagonal axis, resulting in anisotropic and covalent bonding. The charge density is given in units of electrons per primitive cell and the spacing between adjacent contours is 0.5 electrons per primitive cell.

results for this structure are shown. In Sec. III, our results are summarized and the conclusions are presented.

II. CALCULATIONS AND RESULTS

The superconducting transition temperature can be calculated from the McMillan[16] equation if the electron-phonon coupling λ is not too strong ($\lambda \leq 1.25$). In addition to λ, the McMillan equation requires an estimate of the average phonon frequency $\langle\omega\rangle$ and the Coulomb pseudopotential[17] μ^*. In our previous work,[12] an estimate of $\mu^* = 0.10$ was derived, and this value will be assumed here. The average phonon frequency $\langle\omega\rangle$ is defined as

$$\langle\omega\rangle = \frac{\sum_\nu \lambda_\nu(\mathbf{q})\omega_{\mathbf{q}\nu}}{\sum_\nu \lambda_\nu(\mathbf{q})} . \tag{1}$$

The electron-phonon coupling λ used in the McMillan equation can be expressed as a Brillouin-zone average of the wave-vector-dependent coupling $\lambda_\nu(\mathbf{q})$ by

$$\lambda = \sum_\nu \frac{1}{\Omega_{\rm BZ}} \int_{\rm BZ} d\mathbf{q}\, \lambda_\nu(\mathbf{q}), \tag{2}$$

where $\Omega_{\rm BZ}$ is the volume of the Brillouin zone and ν labels the different phonon modes. A first-principles method[18] is used to calculate $\lambda_\nu(\mathbf{q})$ as the double Fermi surface average of the electron-phonon matrix element:

$$\lambda_\nu(\mathbf{q}) = 2N(E_f)\frac{\langle\langle|g(n\mathbf{k}, n'\mathbf{k}', \mathbf{q}\nu)|^2\rangle\rangle}{\hbar\omega_{\mathbf{q}\nu}} , \tag{3}$$

where $\omega_{\mathbf{q}\nu}$ is the phonon frequency for the mode ν with wave-vector $\mathbf{q}$, $N(E_f)$ is the electronic density of states at the Fermi level per atom per spin, and g the electron-phonon matrix element defined by

$$g(n\mathbf{k}, n'\mathbf{k}', \mathbf{q}\nu) = \left(\frac{\hbar\Omega_{\rm BZ}}{2M\omega_{\mathbf{q}\nu}}\right)^{1/2} \left\langle \psi^0_{n\mathbf{k}} \left| \varepsilon_{\mathbf{q}\nu} \cdot \frac{\delta V}{\delta \mathbf{R}} \right| \psi^0_{n'\mathbf{k}'} \right\rangle \delta(\mathbf{k} - \mathbf{k}' - \mathbf{q}) \tag{4}$$

where M is the atomic mass, $\varepsilon_{\mathbf{q}\nu}$ the unit polarization vector, $\delta V/\delta\mathbf{R}$ the change in the self-consistent crystal potential induced by the phonon distortion, and $\psi^0_{n\mathbf{k}}$ and $\psi^0_{n'\mathbf{k}'}$ are the wave functions of the undistorted crystal with wave vectors $\mathbf{k}$ and $\mathbf{k}'$ and band indices n and n'. The difference in total energies between the distorted and undistorted structures is used to calculate $\omega_{\mathbf{q}\nu}$. The change in the self-consistent crystal potential is approximated by

$$\varepsilon_{\mathbf{q}\nu} \cdot \frac{\delta V}{\delta \mathbf{R}} = \frac{V_{\mathbf{q}\nu} - V_0}{\overline{u}_{\mathbf{q}\nu}} , \tag{5}$$

where V_0 and $V_{\mathbf{q}\nu}$ are the self-consistent potentials for the undistorted and distorted crystals, respectively, and $\overline{u}_{\mathbf{q}\nu}$ is the root-mean-square amplitude of the phonon.

The calculation is carried out within a supercell to simplify the evaluation of the Fermi-surface average in Eq. (3). In the supercell method, only wave vectors $\mathbf{q}$ commensurate with the reciprocal lattice ($m\mathbf{q}=\mathbf{G}$, m an integer) can be considered. The main advantage of the supercell method is that in the supercell, $\mathbf{q}$ is a reciprocal lattice vector, so $\mathbf{k}$ and $\mathbf{k}'$ in Eq. (3) are the same point in the Brillouin zone. Even within the supercell method, it is too expensive computationally to calculate $\lambda_\nu(\mathbf{q})$ for more than a few wave vectors $\mathbf{q}$ within the Brillouin zone. Thus, the calculation of λ using Eq. (2) is limited in accuracy by the sparse sampling of the Brillouin zone.

A. Simple hexagonal structure

The sh structure was chosen for a first attempt at calculating T_c for metallic hydrogen in an atomic phase. For this structure, the lattice constant $a = 1.38$ Å and $c/a = 0.6$, corresponding to a Wigner-Seitz radius of 1.3 a.u. or a pressure of 4 Mbar, slightly above the predicted molecular-to-atomic transition pressure. The phonon frequencies calculated for hydrogen in the sh structure are shown in Fig. 2. The center of the Brillouin zone is represented by Γ and the center of its hexagonal faces by A. The center of the rectangular face is denoted by M, and the midpoint of its edge by K. The transversely polarized modes with wave vector along the Γ-A line are found to be unstable from total-energy calculations. Since $c/a < 1$

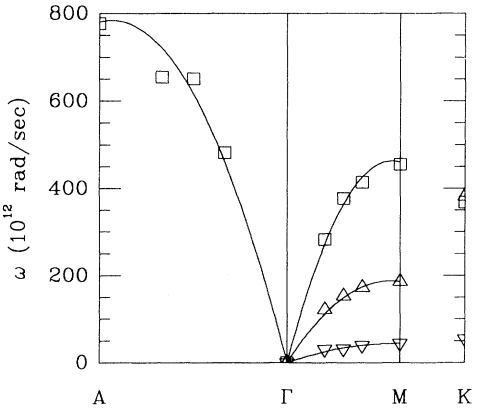

FIG. 2. Phonon dispersion relation $\omega(\mathbf{q})$ for hydrogen in the simple hexagonal structure. Only the longitudinal modes are shown along the Γ-A line, since the transverse modes are unstable. The squares represent longitudinal modes and the triangles represent transverse modes. The lines are drawn as guides to the eye.

in this structure, the nearest neighbors are found along the c axis, and it is not surprising that the longitudinal modes along Γ-A have the highest frequencies of all the modes calculated in the sh structure. Along the Γ-M line and at K, the mode with transverse polarization parallel to the hexagonal axis is particularly soft, reflecting the weak bonding between the "filaments" of charge along the c axis.

The results for $\lambda_\nu(\mathbf{q})$ in the sh structure are shown in Table I. Along the Γ-A line, the transverse modes are unstable and have been omitted from the table. For the other modes listed, the modes labeled "transverse 1" are polarized in the plane (perpendicular to c) while those labeled "transverse 2" are polarized along the hexagonal axis. Since the contributions of different modes to λ vary widely, particularly along the Γ-M line, it is important to study the cause of the variation. The contributions of different modes with widely varying or large $\lambda_{\mathbf{q}\nu}$ can be studied by separating the Fermi-surface average of the matrix element $\langle\langle|g|^2\rangle\rangle$ into the product of a geometric part $\langle\langle 1\rangle\rangle$ and an effective matrix element g_{eff}:

$$\langle\langle|g|^2\rangle\rangle = \langle\langle 1\rangle\rangle|g_{\text{eff}}|^2 , \tag{6}$$

where $\langle\langle 1\rangle\rangle$ represents the double Fermi-surface average of the δ function in Eq. (4), and the remainder of the contributions to $\langle\langle|g|^2\rangle\rangle$ are absorbed into g_{eff}.

The modes along the Γ-M line have a particularly large contribution from the geometric part $\langle\langle 1\rangle\rangle$ due to Fermi-surface nesting, resulting in large $\lambda_{\mathbf{q}\nu}$. The difference between the two transverse modes for these wave vectors results from extremely small matrix elements for the modes polarized parallel to the hexagonal axis.

The averaging of the $\lambda_\nu(\mathbf{q})$ to obtain λ is performed by first spherically averaging along each symmetry direction, and then averaging the contributions to λ from each direction to obtain λ. The spherical average is defined as

$$\lambda_{\nu,\text{avg}} = \left(\sum_{\mathbf{q}} q^2\lambda_\nu(\mathbf{q})\right) \Big/ \sum_{\mathbf{q}} q^2 , \tag{7}$$

where only wave vectors $\mathbf{q}$ along a given symmetry direction are averaged. Averaging along the three symmetry directions yields $\lambda_{\text{avg}}(\Gamma\text{-}A) = 0.34$, $\lambda_{\text{avg}}(\Gamma\text{-}M) = 1.6$, and $\lambda_{\text{avg}}(\Gamma\text{-}K) = 0.7$. Averaging these three numbers results in $\lambda = 0.89$. The average phonon frequency $\langle\omega\rangle$ is calculated by using $\lambda_\nu(\mathbf{q})$ as a weighting factor for each $\omega_{\mathbf{q}\nu}$ and then performing the spherical averaging process described above in Eq. (1). The average phonon frequency is $\langle\omega\rangle = 333 \times 10^{12}$ rad/sec or $\hbar\langle\omega\rangle/k_B = 2540$ K. Together with $\mu^* = 0.10$, the McMillan equation predicts $T_c = 140$ K for hydrogen in the sh structure. This calculation most likely underestimates the value of T_c because the contributions from the transverse modes along Γ-A are not included. In a similar structure where these modes are stable, it is possible that T_c would be substantially higher.

B. Distorted hexagonal structure

Since the sh structure is found to be unstable, we searched for a distorted structure similar to sh that would be stable. Along the Γ-A line in the sh structure, the mode corresponding to a $\mathbf{q} = (0, 0, 2\pi/(3c))$ was substantially more unstable than the other modes studied. This phonon corresponds to a distortion tripling the unit cell along the c axis. The structure found with this distortion "frozen in" is shown in Fig. 3. The layers labeled "A" and "C" have moved to the left and right, respectively, while layers "B" remain stationary. An earlier calculation[12] predicted that hydrogen in this structure would superconduct with a critical temperature $T_c = 230 \pm 85$ K. A more thorough study including more points in the Brillouin zone and better estimates of the

TABLE I. Phonon frequencies $\omega_{\mathbf{q}\nu}$ and electron-phonon coupling $\lambda_{\mathbf{q}\nu}$ for hydrogen in the simple hexagonal structure at 4 Mbar ($a = 1.38$ Å, $c/a = 0.60$) along the Γ-A and Γ-M symmetry directions and at K. The frequencies ω are reported in units of 10^{12} rad/sec. The transverse modes along the Γ-A line are omitted, since they are unstable. For the other symmetry directions, the modes labeled "transverse 1" are polarized perpendicular to the hexagonal axis, while those labeled "transverse 2" are polarized parallel to the hexagonal axis.

$\mathbf{q}$	Longitudinal		Transverse 1		Transverse 2	
	$\lambda_{\mathbf{q}\nu}$	$\omega_{\mathbf{q}\nu}$	$\lambda_{\mathbf{q}\nu}$	$\omega_{\mathbf{q}\nu}$	$\lambda_{\mathbf{q}\nu}$	$\omega_{\mathbf{q}\nu}$
A	0.35	777				
2/3 Γ-A	0.38	654				
1/2 Γ-A	0.21	651				
1/3 Γ-A	0.43	482				
M	0.40	455	1.1	186	0.01	44
2/3 Γ-M	0.44	414	1.2	172	0.01	40
1/2 Γ-M	0.51	377	1.2	153	0.02	32
1/3 Γ-M	0.76	283	1.3	122	0.02	31
K	0.40	368	0.33	381	0.01	54

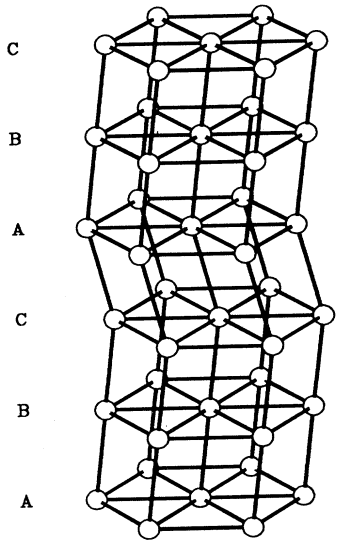

FIG. 3. The distorted simple hexagonal structure (dsh) described in the text. Layers with the same label lie directly above one another and the spacing between the layers is exaggerated for the purpose of clarity. The structure is obtained from the simple hexagonal structure by moving layer A to the left and C to the right while holding layer B fixed.

zone-center (optical) modes reveals that T_c was overestimated due to overcounting of the contribution of modes near the edge of the Brillouin zone and undercounting of the optical modes. The contribution of the optical modes is estimated by calculating λ_ν at the zone center and by assuming that the optical modes do not vary substantially across the zone. In this study, the polarizations of the modes at Γ were calculated by diagonalizing the 9×9 dynamical matrix for $\mathbf{q} = \mathbf{0}$. Of the six optical modes, two were found to be of imaginary frequency; therefore, the dsh structure is also unstable. The transition temperature T_c has been estimated for dsh by including the new points but neglecting the contribution of the unstable modes at the zone center.

Table II shows the results for the dsh structure. Due to poor convergence for the transverse modes with $\mathbf{q}$ along the Γ-A line, only an upper bound for $\lambda_{\mathbf{q}\nu}$ is given for these modes. The wave-vector-dependent electron-phonon coupling $\lambda_{\mathbf{q}\nu}$ is spherically averaged along each symmetry direction and summed over the three polarizations to yield an average λ for each direction (A, L, M, K). The Brillouin zone average in Eq. (2) is defined by

$$\lambda = \lambda_\Gamma + [\lambda_A + \lambda_L + (\lambda_M + \lambda_K)/2]/3 \tag{8}$$

and is found to be $\lambda = 0.97$ if only the four stable modes at the zone center are included and $\lambda = 1.16$ if the contribution of the modes at Γ is multiplied by 1.5 to compensate for the "missing" modes. The average phonon frequency $\langle\omega\rangle$ is calculated to be 326 and 355×10^{12} rad/sec, respectively. The McMillan equation then gives $T_c = 165$ or 233 K, respectively. As with the sh structure, the contributions to λ from different modes vary widely. The phonons with wave vector two-thirds of the way from Γ to M provide the strongest single contribution to λ due to Fermi surface nesting. If they are omitted from the average, λ drops by 0.08 and T_c falls to

TABLE II. Phonon frequencies $\omega_{\mathbf{q}\nu}$ and electron-phonon coupling $\lambda_{\mathbf{q}\nu}$ for hydrogen in the distorted simple hexagonal (dsh) structure described in the text. The frequencies ω are reported in units of 10^{12} rad/sec. The four stable optical modes at Γ are shown. For the modes along Γ-A, the transverse 1 and 2 modes are polarized parallel to and perpendicular to the distortion, respectively. For the modes at K and along Γ-M, the transverse 1 mode is polarized perpendicular to the hexagonal c axis, while the transverse 2 mode is polarized parallel to c. Along Γ-L, the three polarizations are in the three Cartesian directions x,y,z, respectively. Only an upper limit on $\lambda_{\mathbf{q}\nu}$ could be found for the transverse modes of wavevector 2/3 A; see the text for discussion.

q	Longitudinal		Transverse 1		Transverse 2	
	$\lambda_{\mathbf{q}\nu}$	$\omega_{\mathbf{q}\nu}$	$\lambda_{\mathbf{q}\nu}$	$\omega_{\mathbf{q}\nu}$	$\lambda_{\mathbf{q}\nu}$	$\omega_{\mathbf{q}\nu}$
Γ	0.15	589	0.02	198		
	0.16	561	0.06	62		
A	0.13	443	0.17	114	0.05	73
2/3 Γ-A	0.22	314	<0.25	57	<0.25	28
M	0.13	331	0.35	195	0.04	62
2/3 Γ-M	0.20	400	1.5	97	0.42	140
L	0.08	399	0.53	168	0.13	455
2/3 Γ-L	0.11	398	0.47	167	0.13	301
K	0.13	372	0.10	377	0.16	86

150 or 220 K, respectively. We therefore estimate that the uncertainty in our calculated λ and $\langle\omega\rangle$ is on the order of 10%; thus, if the dsh structure were stable, it would be superconducting with T_c between 150 and 230 K, rather than between 150 and 300 K as predicted earlier.

C. 9R and α-Te structures

Since the dsh structure is also unstable, we have once again searched for a stable structure. Preliminary calculations indicate that within the constraint of a three-atom primitive cell, a structure very similar to that of α-Te is stable. The α-Te structure consists of hexagonal planes with a threefold screw axis perpendicular to the planes, and the space group is D_3^4.

A more promising candidate for the structure of atomic metallic hydrogen is the 9R or $\alpha-$Sm structure, which is the low-temperature structure of lithium. The 9R structure is a rhombohedral structure with a basis containing three atoms. It can be described as a stacking of hexagonal planes in the sequence $[\cdots ABACACBCB\cdots]$ repeating every nine layers — hence the name 9R. Figure 4 shows both the stacking of the hexagonal layers and the rhombohedral unit cell. Since hydrogen under pressure is predicted to be a monovalent metal, the structures of the alkali metals may be good candidate structures for atomic metallic hydrogen. Total-energy calculations indicate that for pressures near 4 Mbar, the 9R structure is energetically competitive with the simple hexagonal structure found earlier. The energy difference between the two structures is within the uncertainty imposed by the calculation; therefore, we cannot authoritatively state whether 9R or sh is more stable. For $r_s = 1.3$ a.u., we find that the most favorable c/a ratio for this structure is 1.41 times the ideal ratio $c/a = 6^{1/2}$.

Table III shows the results for the wave-vector-dependent electron-phonon coupling $\lambda_\nu(\mathbf{q})$ and phonon frequencies $\omega_{\mathbf{q}\nu}$ for three symmetry points in the Brillouin zone. The point Γ is at the center of the zone, L is at the center of a face of the zone and corresponds to one-half of a primitive reciprocal lattice vector, and T is the point along the c axis that corresponds to A in the hexagonal Brillouin zone. Adding the contribution from the modes at each $\mathbf{q}$ together yields $\lambda_\Gamma = 0.37$, $\lambda_L = 2.37$,

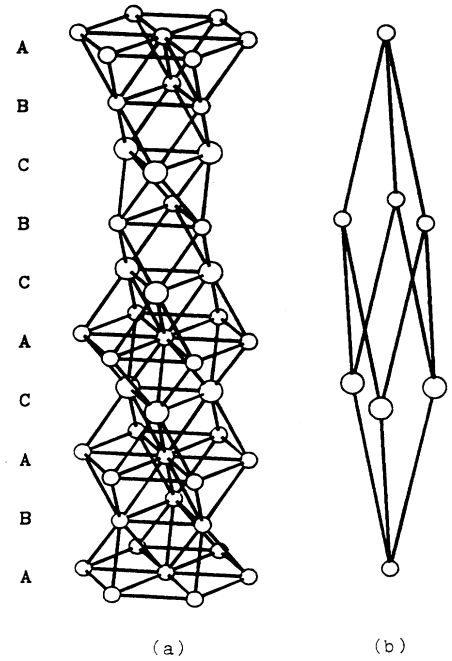

FIG. 4. The 9R structure described in the text. The structure can be viewed as either rhombohedral with a basis of three atoms or as hexagonal layers with the stacking sequence $[\cdots ABACACBCB\cdots]$. The hexagonal layers are shown in (a). For the layers in the A position, seven atoms are shown. The B and C layers have only three atoms, and the C layers are distinguished by larger atoms. The rhombohedral unit cell is shown in (b). The basis consists of three atoms at $(0,0,0)$ and $\pm(\frac{2}{9},\frac{2}{9},\frac{2}{9})$.

TABLE III. Phonon frequencies $\omega_{\mathbf{q}\nu}$ and electron-phonon coupling $\lambda_{\mathbf{q}\nu}$ at the symmetry points Γ, L, and T for hydrogen in the 9R phase described in the text. The modes are labeled by the irreducible representation to which they belong. At the T point, the modes labeled (D) are doubly degenerate and enter into the averaging process twice. The frequencies ω are reported in units of 10^{12} rad/sec.

q	ν	$\lambda_{\mathbf{q}\nu}$	ω
Γ	Γ_{3u}	0.02	40
	Γ_{3u}	0.02	40
	Γ_{2u}	0.16	456
	Γ_{3g}	0.01	42
	Γ_{3g}	0.01	41
	Γ_{1g}	0.15	455
L	L_{1g}	0.10	423
	L_{1g}	0.23	237
	L_{1u}	0.34	160
	L_{2g}	0.35	159
	L_{2g}	0.02	153
	L_{2u}	0.25	432
	L_{2u}	0.16	210
	L_{2u}	0.27	162
	L_{2u}	0.67	147
T	T_{1g}	0.33	258
	$T_{3g}(D)$	0.04	23
	T_{2u}	0.17	440
	T_{2u}	0.33	257
	$T_{3u}(D)$	0.02	49
	$T_{3u}(D)$	0.04	20

and $\lambda_T = 0.93$. Averaging these three together with equal weights yields $\lambda = 1.22$. If λ_Γ is averaged with both of λ_L and λ_T, $\lambda_{\Gamma\text{-}L} = 1.37$ and $\lambda_{\Gamma\text{-}T} = 0.65$ are obtained. Averaging these yields $\lambda = 1.01$. These values for λ are taken as bounds on the actual value of λ for the $9R$ structure. The average phonon frequency $\langle\omega\rangle$ is calculated as described above and varies from 240×10^{12} to 254×10^{12} rad/sec, or from 1830 to 1940 K. Using the estimate of $\mu^* = 0.10$, the McMillan equation predicts that T_c should be between 135 and 170 K.

III. CONCLUSIONS

The hexagonal structures studied here are candidates for the most stable structure of atomic metallic hydrogen at 4 Mbar. The simple hexagonal structure and a distorted simple hexagonal structure discussed earlier are found to be unstable. More detailed calculations of the electron-phonon coupling in the dsh structure show that the earlier calculation overestimated the transition temperature T_c, and a better estimate is that T_c for hydrogen in this structure lies between 150 and 230 K. The $9R$ structure has also been examined as a candidate for the atomic structure of hydrogen, and the critical temperature for hydrogen in this structure is predicted to lie between 135 and 170 K.

A summary of the results is presented in Table IV and Fig. 5. For all the structures considered, we find that T_c falls between 120 and 230 K, with the electron-phonon coupling λ lying between 0.80 and 1.22. The value of λ for the free-electron model (jellium) is much smaller than those for the structures considered because of local field effects due to covalent bonding, while the high $\langle\omega\rangle$ found for jellium originates in the use of a Debye model for the phonon spectrum. Figure 5 shows T_c as a function of λ for several values of the average phonon frequency $\langle\omega\rangle$ using the McMillan equation and $\mu^* = 0.10$. In all three structures, the electron-phonon coupling λ is in the neighborhood of 1.0. For the characteristic phonon frequencies $\langle\omega\rangle$ found for hydrogen in the three structures considered here, T_c is then found to be in the range of 130–170 K.

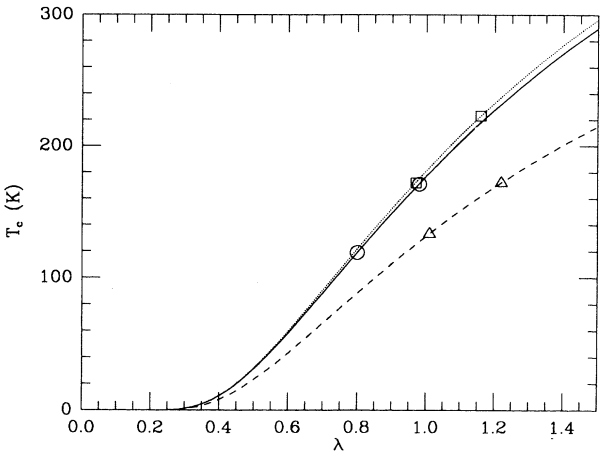

FIG. 5. Transition temperature T_c as a function of coupling strength λ for several values of $\langle\omega\rangle$ corresponding to those found for the three structures considered. The McMillan equation is used to calculate T_c. Results for the simple hexagonal (solid line), dsh (dotted line), and $9R$ structures (dashed line) are shown. Also shown are the calculated upper and lower values of T_c for the sh structure (circles), dsh structure (squares), and the $9R$ structure (triangles) based on the uncertainty in λ. The T_c values calculated for all structures considered lie between 130 and 230 K.

If the actual structure of metallic hydrogen should differ greatly, the value of T_c could be substantially different. However, in all three candidate structures presented here, we find that hydrogen is a high-temperature superconductor, so it is likely that atomic metallic hydrogen will superconduct at temperatures in the range of 120–230 K.

TABLE IV. Summary of predicted T_c values for hydrogen in the structures discussed in the text. The upper and lower bounds for T_c are shown for each structure along with the electron-phonon coupling λ and the average phonon frequency $\langle\omega\rangle$. For comparison, the value of λ for a free-electron model (FEM) using Thomas-Fermi screening is also given. For the FEM, $\langle\omega\rangle$ is estimated using a Debye model for the phonon spectrum. The McMillan equation is used together with an estimate of the Coulomb pseudopotential $\mu^* = 0.10$ to calculate T_c. For all the structures considered, T_c lies between 120 and 230 K.

Structure	λ	$\langle\omega\rangle$ (10^{12} rad/sec)	T_c (K)
sh(low)	0.80	333	120
sh(high)	0.98	333	170
dsh(low)	0.97	326	165
dsh(high)	1.16	355	230
$9R$(low)	1.01	240	135
$9R$(high)	1.22	254	170
FEM	0.60	825	144

Future studies will examine the electron-phonon coupling for the α-Te structure mentioned above, as well as the possibility of superconductivity in the *molecular* metallic (band-overlap) phase of hydrogen.

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