Erratum: High-temperature superconductivity in atomic metallic hydrogen [Phys. Rev. B 84, 144515 (2011)]

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(Received 26 May 2012; published 19 June 2012)

DOI: 10.1103/PhysRevB.85.219902 PACS number(s): 74.20.Pq, 74.10.+v, 74.62.Fj, 74.20.Fg, 99.10.Cd

In Ref. 1, herein referred to as *I*, labels designating the crystal structures under consideration were omitted from some figures, which could be a source of confusion. Moreover, superconducting parameters necessary to estimate critical temperatures, T_c, were calculated using the nonweighted phonon density of states, $F(\omega)$, rather than the proper normalized weighting function of the Eliashberg theory,[2] $g(\omega)$.

In this Erratum, we first review the theoretical background for calculating the parameters needed to estimate T_c, in particular their evaluation using $g(\omega)$. We then present and discuss results analogous to Figs. 4, 5, and 13 of *I* with revised calculations and including crystal-structure labels. Finally, we provide a brief summary of the differences between calculations.

In order to evaluate the McMillan formula[2,3] or the Allen-Dynes equation[4] to estimate T_c, Eqs. (2) and (3) of *I*, respectively, we must determine λ, $\langle\omega\rangle$, $\bar{\omega_2}$, $\omega_{\ln}$, and μ^*; these correspond to the attractive electron-phonon-induced interaction, the first and square root of the second moments of $g(\omega)$, the logarithmic average phonon frequency [i.e., $\ln(\omega_{\ln}) = \langle \ln \omega \rangle$], and the renormalized Coulomb repulsion, respectively. As in *I*, below we take the approximate, yet reasonable,[5] value of 0.089 for μ^*. Further, λ is a direct measure of the strength of the electron-phonon spectral function $\alpha^2F(\omega)$, which is readily calculable via *ab initio* calculations,[6]

$$\lambda = 2\int_0^\infty d\omega\, \alpha^2 F(\omega)/\omega. \tag{1}$$

$\langle\omega\rangle$, $\bar{\omega_2}$, and $\omega_{\ln}$ can also be calculated directly from $\alpha^2F(\omega)$,

$$\langle\omega\rangle = \int_0^\infty d\omega\, g(\omega)\,\omega, \tag{2}$$

$$\bar{\omega_2} = \left[\int_0^\infty d\omega\, g(\omega)\,\omega^2\right]^{1/2}, \tag{3}$$

$$\omega_{\ln} = \exp\left[\int_0^\infty d\omega\, g(\omega)\ln(\omega)\right], \tag{4}$$

where

$$g(\omega) = \frac{2}{\lambda\omega}\alpha^2 F(\omega). \tag{5}$$

The difference between Eqs. (2)–(4) and those presented and used in *I* is via the use of $g(\omega)$ in place of $F(\omega)$, which results in weighted averages. λ, $\langle\omega\rangle$, and $\omega_{\ln}$ calculated using Eqs. (1), (2), and (4), as well the corresponding estimates of T_c calculated using Eqs. (2) and (3) of *I*, are presented and discussed below.

λ. The use of $g(\omega)$ in Eqs. (2)–(4) does not affect the calculation of λ. Nonetheless, in Fig. 1, we show again λ values for both the $I4_1/amd$ and R-3m structures[7] considered in *I*, but we now include crystal-structure labels.

Note that values for R-3m are not shown between ∼1 and 2 TPa (as in *I*), because of complications in applying Eqs. (2)–(4) in the presence of (unphysical) imaginary phonon frequencies (see below).

$\langle\omega\rangle$ and $\omega_{\ln}$. Temperature prefactors $\langle\omega\rangle/k_B$ and $\omega_{\ln}/k_B$, where k_B is Boltzmann's constant, calculated using Eqs. (2)–(4), including crystal-structure labels, are shown in Fig. 2.

As in *I*, $\langle\omega\rangle$ and $\omega_{\ln}$ both exhibit similar trends with pressure, the latter at a slightly lower magnitude. Further, when $g(\omega)$ is used in Eqs. (2) and (4) instead of $F(\omega)$, there is a decrease in the magnitudes of both (compare, for example, directly with Fig. 4 of *I*). At relatively low pressure, there is only a minor difference (e.g., the prefactors are ∼2000 K near 500 GPa, as opposed to ∼2200 K). As the pressure is increased, however, which causes the phonon frequencies to move correspondingly higher, the difference becomes greater (e.g., at 3 TPa, the prefactors become ∼2250 K, as opposed to 3600 K). This latter result suggests that the corresponding T_c values will be somewhat reduced as well (see below).

We note that values are not shown for pressures near 1–2 TPa for R-3m. This is a consequence of the (classically predicted) instabilities in this pressure range.[1,7] For a classically unstable structure, imaginary phonon frequencies can appear in the phonon dispersion. Because of this, $\alpha^2F(\omega)$ becomes finite as $\omega \to 0$, and this causes an unbound and unphysical increase in $g(\omega)$ (see also Figs. 10 and 11 of *I*).

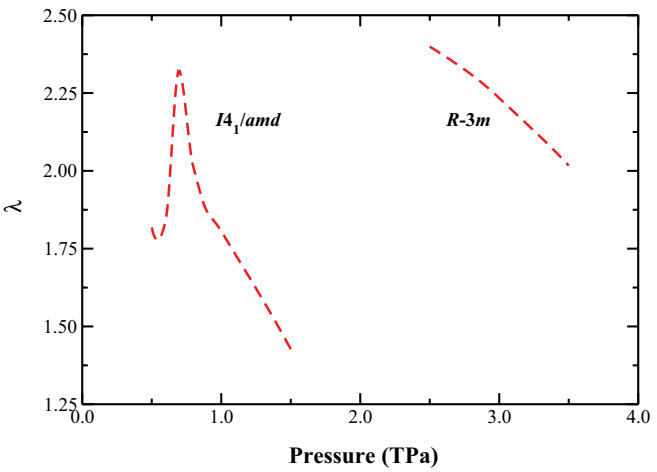

FIG. 1. (Color online) Electron-phonon-induced interaction, λ, as a function of pressure.

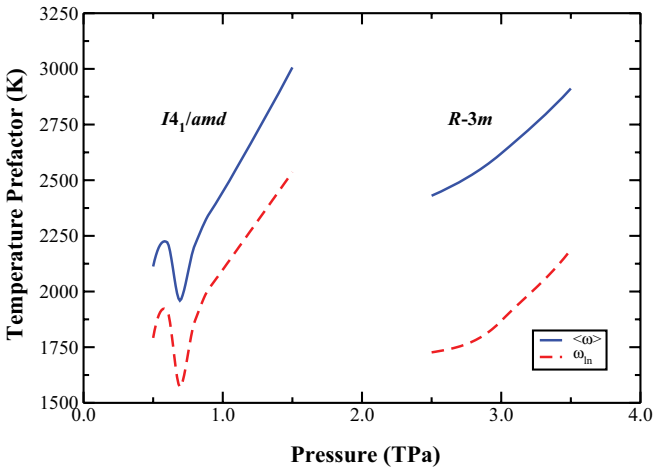

FIG. 2. (Color online) Temperature prefactors $\langle\omega\rangle/k_B$ (solid blue line) and ω_{ln}/k_B (dashed red line) as a function of pressure.

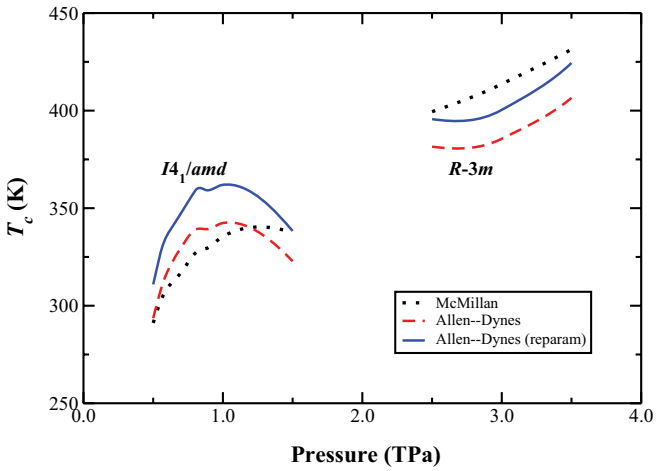

FIG. 3. (Color online) Superconducting critical temperatures, T_c, calculated using Eqs. (2) and (3) of *I*, as a function of pressure.

Equations (2)–(4), under such circumstances, cannot therefore be reliably evaluated.

T_c. Estimated T_c values calculated using the weighted superconductivity parameters in Eqs. (2)–(4), including crystal-structure labels, are shown in Fig. 3.

As expected, the estimated T_c values are somewhat reduced compared to those in *I*. Nonetheless, the qualitative physics remains the same. Near molecular dissociation (∼500 GPa), superconductivity is still predicted to occur above room temperature. As the pressure is increased and the atomic phase stabilizes, T_c increases. However, in contrast to the results reported in *I*, T_c is predicted to only reach ∼360 K, as opposed to 481 K. Further, at the atomic-atomic structural phase transformation ($I4_1/amd \rightarrow R\text{-}3m$), T_c is still expected to increase. While we cannot reliably estimate T_c precisely near 1–2 TPa, as discussed above, we can infer this based on the large T_c values at higher pressure (e.g., near 3 TPa, T_c approaches 425 K).

In conclusion, we presented results to replace Figs. 4, 5, and 13 of *I*. The new figures contain crystal-structure labels to prevent possible confusion, as well as revised and more reliable (properly calculated) values of $\langle\omega\rangle$, ω_{ln}, and T_c. While some differences in results exist relative to those reported in *I*, their qualitative features remain unchanged. In particular, T_c values (Fig. 3) remain remarkably high, above room temperature, which continues to suggest the interesting possibility that the atomic phase of hydrogen exists entirely in a superconducting state.

We thank N. W. Ashcroft for pointing out the lack of crystal-structure labels in some figures of *I*.

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