The discovery of superconductivity in MgB$_2$ (Refs. 1 and 2) has renewed interest$^{3-11}$ in finding superconductivity in similar materials such as simple metal diborides [BeB$_2$, BeB$_2$$_{7.75}$ (Ref. 3)], transition-metal diborides [NbB$_2$ (Refs. 4, 5), TaB$_2$ (Refs. 4, 6), MoB$_2$ (Ref. 7), ZrB$_2$ (Ref. 8)], borocarbides [LiBC$_2$ (Refs. 9, 10)], and other alloys.$^{11}$ Surprisingly, many of the materials mentioned above have not shown any superconductivity; those that are found to superconduct do so at a relatively low $T_c$<10 K, and, very likely, require hole doping and/or external pressure to show superconductivity. For example, the recent work of Yamamoto et al.$^9$showing superconductivity in hole-doped NbB$_2$ is a case in point. Thus, of all the diborides, MgB$_2$ seems to be in a class by itself with a $T_c=39$ K while all the other diborides have $T_c<10$ K.

Recent work on MgB$_2$ (Refs. 12–20) has unambiguously shown a very strong and anisotropic electron-phonon coupling in this system. In particular, it is found that electron-hole states on the cylindrical sheets of the Fermi surface along $\Gamma$-$A$ couple very strongly to the in-plane $B$-$B$ bond stretching $E_{2g}$ phonon mode.$^{15-19}$ The $E_{2g}$ phonon-mode coupling gives rise to partial electron-phonon coupling constant $\lambda_q$ of the order of 2–3.$^{19}$ Such a large partial $\lambda_q$ along $\Gamma$-$A$ results in a relatively high superconducting transition temperature of 39 K. Thus, the observed differences in the superconducting properties of MgB$_2$ in relation to other diborides, especially the transition-metal diborides, can be better understood by comparing the electron-phonon coupling along $\Gamma$-$A$ in these systems. Taking the cue, we have studied from first principles (i) the phonon dispersion $\omega_q$, (ii) the phonon linewidth $\gamma_q$, and (iii) the partial electron-phonon coupling constant $\lambda_q$ along $\Gamma$-$A$ in MgB$_2$, NbB$_2$, and TaB$_2$ in $P6/mmm$ crystal structure.

We have calculated the electronic structure of MgB$_2$, NbB$_2$, and TaB$_2$ in $P6/mmm$ crystal structure. We used optimized lattice constants $a$ and $c$ for MgB$_2$ and NbB$_2$ (Ref. 20), and experimental lattice constants ($a=5.826$ a.u., $c=6.130$ a.u.) for TaB$_2$ which are close to our optimized values of $a=5.792$ a.u. and $c=6.143$ a.u. The lattice constants were optimized using the ABINIT program$^{22}$ based on pseudopotentials and plane waves. For studying the electron-phonon interaction we used the full-potential linear response program of Savrasov$^{23,24}$ to calculate the dynamical matrices and the Hopfield parameter, which were then used to calculate the phonon dispersion $\omega_q$, the phonon linewidth $\gamma_q$, and the partial electron-phonon coupling constant $\lambda_q$ along $\Gamma$-$A$ in MgB$_2$, NbB$_2$, and TaB$_2$.

Based on our calculations, described below, we find that (i) in contrast to a strong and $E_{2g}$-mode-dominated electron-phonon coupling in MgB$_2$, the transition-metal diborides NbB$_2$ and TaB$_2$ have a relatively weak electron-phonon coupling which is dominated by the longitudinal acoustical (LA) mode, (ii) the $E_{2g}$ phonon linewidth is an order of magnitude larger in MgB$_2$ than in NbB$_2$ or TaB$_2$, and (iii) the $E_{2g}$ frequency in NbB$_2$ and TaB$_2$ is considerably higher than in MgB$_2$ while the LA phonon frequency at $A$ for TaB$_2$ is almost half of that of MgB$_2$ or NbB$_2$.

Before describing our results in detail, we provide some of the computational details. As indicated above, the structural relaxation was carried out by the molecular dynamics program ABINIT (Ref. 22) with Broyden-Fletcher-Goldfarb-Shanno minimization technique using the Troullier-Martins pseudopotential$^{25}$ for MgB$_2$ and Hartwigsen-Goedecker-Hutter pseudopotentials$^{26}$ for NbB$_2$ and TaB$_2$, 512 Monkhorst-Pack$^{27}$ k points, and Teter parametrization for exchange correlation. The kinetic energy cutoff for the plane waves was 110 Ry for MgB$_2$ and 140 Ry for NbB$_2$ and TaB$_2$. The charge self-consistent full-potential linear muffin-tin orbital$^{28}$ (LMTO) calculations for electronic structure were carried out with the generalized gradient approximation for exchange correlation of Perdew et al.$^{28}$ and 484 k points in the irreducible wedge of the Brillouin zone. In these calculations, we used $s$, $p$, $d$, and $f$ orbitals at the Mg and Ta sites and $s$, $p$, and $d$ orbitals at the Nb and B sites. The 2$p$ state of Mg and the 5$s$ and 5$p$ states of Ta were treated as semicore states. In all cases the potential and wave function were expanded up to $l_{max}=6$. The muffin-tin radii for Mg, B, Nb, and Ta were taken to be 2.4, 1.66, 2.3, and 2.5 a.u., respectively.

The calculation of dynamical matrices and the Hopfield parameters along $\Gamma$-$A$ was carried out for four equidistant q points for MgB$_2$ and seven equidistant q points for NbB$_2$ and TaB$_2$. For Brillouin zone integrations we used a 12$x$12 grid while the Fermi surface was sampled more accurately with a 36$x$36$x$36 grid of k points using the double-grid technique as outlined in Ref. 24. We checked the con-
vergence of the relevant quantities by carrying out Brillouin zone integrations using a $16 \times 16 \times 16$ grid of $k$ points with Fermi surface sampling done over $48 \times 48 \times 48$ grid.

In Fig. 1 we show the phonon dispersion of MgB$_2$, NbB$_2$, and TaB$_2$ for LA and optical $E_{2g}$ modes along $\Gamma$-$A$. For MgB$_2$, a comparison of our calculations of $E_{2g}$ and LA phonon frequencies at $\Gamma$ and $A$ points with the previous calculations of Refs. 15, 16, and 19 is given in Table I. As expected, our results are closer to the work of Ref. 15. The difference in the $E_{2g}$ phonon frequency at $\Gamma$, which has been found to be very sensitive to the structural input and Brillouin zone integration, arises due to the experimental lattice constants used in Refs. 15, 16, and 19. The value calculated by Shukla et al. for the $E_{2g}$ phonon frequency is somewhat lower. However, our calculated frequency for the LA phonon mode at $A$ is in good agreement with previous calculations. We expect $\omega(q_A)$ for NbB$_2$ and TaB$_2$ to have similar accuracy.

In NbB$_2$ and TaB$_2$, the $E_{2g}$ phonon mode along $\Gamma$-$A$ has considerably stiffened in comparison with MgB$_2$. The $E_{2g}$ frequency in MgB$_2$ changes from 78 to 72 meV, while for NbB$_2$ and TaB$_2$ it changes from 110 to 107 meV and from 108 to 105 meV from $\Gamma$ to $A$, respectively. The $E_{2g}$ frequency at $\Gamma$ in TaB$_2$, as calculated by Rosner et al.,$^{29}$ is 98 meV. The LA phonon mode at $A$ for TaB$_2$ (22 meV) is almost half of that of MgB$_2$ (40 meV) and NbB$_2$ (37 meV). Here, we like to point out that in the present work the number of $k$ points chosen along $\Gamma$-$A$ is not sufficient to say anything about the anomaly in the acoustical mode.

The differences in the nature of electron-phonon interaction between MgB$_2$ and the transition-metal diborides NbB$_2$ and TaB$_2$ become quite apparent if one considers the electron-phonon contribution to the phonon lifetimes. In the case of MgB$_2$, as shown by Shukla et al.,$^{19}$ anharmonic effects make negligible contribution to the phonon linewidth. Thus, the anomalous broadening of the $E_{2g}$ phonon linewidth along $\Gamma$-$A$ underscores the strength of the electron-phonon coupling for this particular mode in MgB$_2$.$^{19}$ To see what happens in the transition-metal diborides, we show in Fig. 2 the phonon linewidths of MgB$_2$, NbB$_2$, and TaB$_2$ for LA and $E_{2g}$ modes along $\Gamma$-$A$. For MgB$_2$, our calculated $\gamma_{\omega}$’s are in reasonable agreement with the results of Ref. 19. Note that the values shown in Fig. 2 correspond to twice the linewidth. From Fig. 2, it is clear that in MgB$_2$ the electron-phonon coupling along $\Gamma$-$A$ is dominated by the optical $E_{2g}$ phonon mode with a maximum $\gamma_{E_{2g}}$ of 44 meV and that the LA mode plays essentially no role. In contrast, in NbB$_2$ and TaB$_2$ (i) the linewidths are more than an order of magnitude smaller than in MgB$_2$—for example, the maximum $\gamma_{E_{2g}}$ is only about 4 meV in TaB$_2$—(ii) the contribution from the $E_{2g}$ mode decreases from 4 to 2.8 meV, while that due to the LA mode increases from 0.02 to 1.5 meV, as one moves from $\Gamma$ to $A$. The phonon linewidths of MgB$_2$ and the transition-metal diborides NbB$_2$ and TaB$_2$, as described above, clearly demonstrate the differences in the strength and the nature of the electron-phonon interaction in these systems.

To see the strengths with which the LA and the $E_{2g}$ phonon modes couple to the electrons, we show in Fig. 3 the

![FIG. 1. The phonon dispersion $\omega(q_A)$ of MgB$_2$ (upper panel), NbB$_2$ (middle panel), and TaB$_2$ (lower panel) for longitudinal acoustical (solid circles connected with solid line) and optical $E_{2g}$ (open circles connected with dashed line) modes along $\Gamma$-$A$, calculated using the full-potential linear response method as described in the text. The lines connecting the points are only a guide to the eye.](image1)

![FIG. 2. The phonon linewidth $\gamma_{\omega}$ of MgB$_2$ (upper panel), NbB$_2$ (middle panel), and TaB$_2$ (lower panel) for LA (solid bar) and optical $E_{2g}$ (open bar) modes along $\Gamma$-$A$, calculated using the full-potential linear response method as described in the text. The phonon linewidth for the LA mode in MgB$_2$ has been multiplied by a factor of 10 for clarity.](image2)

![TABLE I. The phonon frequencies (in meV) at $\Gamma$ and $A$ for the $E_{2g}$ and LA modes for MgB$_2$ calculated using the linear response method as described in the text as well as from previous work.](table1)

<table>
<thead>
<tr>
<th></th>
<th>$\omega_{\Gamma}(E_{2g})$</th>
<th>$\omega_{A}(E_{2g})$</th>
<th>$\omega_{A}(LA)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Present work</td>
<td>78</td>
<td>72</td>
<td>40</td>
</tr>
<tr>
<td>Kong et al.$^a$</td>
<td>73</td>
<td>71</td>
<td>38</td>
</tr>
<tr>
<td>Bohnen et al.$^b$</td>
<td>71</td>
<td>63</td>
<td>39</td>
</tr>
<tr>
<td>Shukla et al.$^c$</td>
<td>65</td>
<td>57</td>
<td>37</td>
</tr>
</tbody>
</table>

$^a$Reference 15.
$^b$Reference 16.
$^c$Reference 19.
partial as well as the total electron-phonon coupling constant ($\lambda_q$) along $\Gamma$-$A$ for MgB$_2$, NbB$_2$, and TaB$_2$. Certainly, the most striking feature of these systems, as evidenced in Fig. 3, is the overall strength of the electron-phonon coupling in MgB$_2$ ($\lambda_q \approx 7.9$) as compared to NbB$_2$ ($\lambda_q \approx 1.5$) and TaB$_2$ ($\lambda_q \approx 2.5$); nevertheless, the additional feature of $E_{2g}$-dominated $\lambda_q$ in MgB$_2$ giving way to LA-dominated $\lambda_q$ in NbB$_2$ and TaB$_2$ is just as striking. Thus, the electron-phonon coupling in the transition-metal diborides NbB$_2$ and TaB$_2$ is essentially due to the LA mode (the transverse acoustical mode makes some contribution), the contribution from the $E_{2g}$ mode being insignificant. For TaB$_2$, Rosner et al.\textsuperscript{29} also found $\lambda_{E_{2g}} = 0.05$ at $\Gamma$, in agreement with the present work. However, their\textsuperscript{29} conclusion about the strength of the electron-phonon coupling in TaB$_2$ is erroneous because it does not take into account the contributions from the acoustical modes properly. We also note that, in our opinion,\textsuperscript{20,30} the experimentally\textsuperscript{31} deduced electron-phonon coupling in NbB$_2$ and TaB$_2$ is underestimated. These differences in the electron-phonon coupling between MgB$_2$ and the transition-metal diborides NbB$_2$ and TaB$_2$ may help explain why MgB$_2$ superconducts at 39 K while NbB$_2$ and TaB$_2$ do not show any superconductivity down to 2 K.

Finally, in Fig. 4 we show the convergence of $\omega_q$, $\gamma_q$, and $\lambda_q$ at $A$ in the Brillouin zone for NbB$_2$ as a function of $\mathbf{k}$ points using the double-grid technique as outlined in Ref. 24. The use of the double-grid technique allows one to construct two separate but commensurate $\mathbf{k}$ grids, one for the electronic charge self-consistency and the other for Fermi surface sampling. We employed four sets of double grids (i) (8, 8, 8, 24), (ii) (12, 12, 12, 24), (iii) (12, 12, 12, 36), and (iv) (16, 16, 16, 48), where the first three numbers define the electronic self-consistency grid and the last number specifies the Fermi surface sampling grid which is commensurate with the first grid. We find that the results are converged for the (12,12,12,36) grid used in the present work.

In conclusion, we have studied from first principles (i) the phonon dispersion, (ii) the phonon linewidth, and (iii) the partial electron-phonon coupling constant along $\Gamma$-$A$ in MgB$_2$, NbB$_2$, and TaB$_2$ in $P6/mmm$ crystal structure. We find that (i) in contrast to a strong and $E_{2g}$-mode-dominated electron-phonon coupling in MgB$_2$, the transition-metal diborides NbB$_2$ and TaB$_2$ have a relatively weak electron-phonon coupling which is dominated by the LA mode, (ii) the $E_{2g}$ phonon linewidth is an order of magnitude larger in MgB$_2$ than in NbB$_2$ or TaB$_2$, and (iii) the $E_{2g}$ phonon frequency in NbB$_2$ as well as TaB$_2$ is considerably higher in MgB$_2$ while the LA phonon frequency at $A$ for TaB$_2$ is almost half of that of MgB$_2$ or NbB$_2$.