Electron–phonon interaction and superconductivity in hexagonal ternary carbides Nb$_2$AC ($A$: Al, S, Ge, As and Sn)

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**Keywords**: superconductivity, MAX phase, electronic structure, electron–phonon coupling, DFT, ab initio

Supplementary material for this article is available online

**Abstract**

The superconducting transition temperatures $T_c$ of hexagonal Nb$_2$AC ($A$: Al, S, Ge, As and Sn) are investigated using density functional perturbation theory to model the electron–phonon interaction. A critical assessment of the calculated electronic structure and density of states revealed that the electronic states near to the Fermi level are mostly composed of the Nb 4d states, which are responsible for the electrical conductivity. The theoretical $T_c$ data from electron–phonon calculations are in excellent agreement with the Fröhlich model, and this model was used as a computationally efficient screening method to identify promising Nb–C$_2$M$_2$AX phase materials.

For Nb$_2$AC ($A$: Zn, Cd, Al, Ga, In, Tl, Si, Pb and P), the model indicated that Nb$_2$AlC should have the highest $T_c$ of this set, a little lower than Nb$_2$GeC and comparable to Nb$_2$SC and Nb$_2$SnC. Superconductivity in Nb$_2$AlC has not been studied experimentally, but this result was confirmed by full electron–phonon calculations, which also revealed that the mechanism for superconductivity is the interactions of Nb 4d-state electrons with low-frequency phonons (in particular, acoustic phonon and low-frequency optical phonons dominated by Nb and the $A$ element). The average electron–phonon coupling parameter was found to be $\lambda \sim 0.646, 0.739, 0.685, 0.440$ and $0.614$ for Nb$_2$AC ($A$: Al, S, Ge, As and Sn), respectively, with a corresponding superconducting critical temperature $T_c \sim 6.7$ K, 7.7 K, 9.8 K, 2.1 K and 6.3 K, respectively.

1. Introduction

Metal carbides and carbonitrides are extraordinary materials that demonstrate outstanding properties, such as high hardness, ultra-high temperature stability, creep resistance, high electrical and thermal conductivity, paramagnetic properties and photoluminescence, so they have attracted considerable attention in the last few years and several technical applications have been reported [1–4]. In recent years, $M_2AX$ phases, where $M$ is an early transition metal from group 3 (Sc, Lu), 4 (Ti, Zr, Hf), 5 (V, Nb, Ta), 6 (Cr, Mo), or 7 (Mn), $A$ is an element from group 12 (Zn, Cd), 13 (Al, Ga, In, Tl), 14 (Si, Ge, Sn, Pb), 15 (P, As), or 16 (S) and $X$ is C or N, have been extensively studied because they exhibit a curious combination of properties usually associated with both metals and ceramics. Like metals, they are electrically and thermally conductive, not susceptible to thermal shock, plastic at high temperature, exceptionally damage tolerant and readily machinable [5–12]. Like ceramics, they have high hardness, high creep lifetime, high oxidation resistance and thermal fatigue endurance [13–20]. These unique properties make them suitable for applications as advanced materials in many different technologies and under extreme conditions, including high temperature, high pressure or nuclear radiation environments [21]. Furthermore, $M_2AX$ phases have the potential to be used for coating on spacecraft to prohibit solar heating [22]. In addition, some of the $M_2AX$ phases are known to be low temperature superconductors. Low temperature superconductors are also of considerable interest with many applications, for example, superconducting coils make possible the very powerful electromagnets used in fundamental research
as well as in applications such as magnetic resonance imaging and Maglev trains. In addition, low-temperature superconductors have been used for superconducting memory, cables, current limiters and very sensitive magnetic field detectors (SQUIDs) etc [23–25].

In 1967, Jeitschko reported on the fabrication and characterization of Ti2AlN [26] from which the M2AX phase family has grown. So far, nearly 40 M2AX phases have been synthesized, and ten of them have been found experimentally to be low transition temperature superconductors: Mo2GaC [27], Nb5SC [28], Nb2AsC [29], Nb2SnC [30], Ti2InC [31], Nb2InC [32], Ti2InN [32], Ti2GeC [34], Lu2SnC [35] and Nb2GeC [36]. The discovery of superconductivity in these materials has inspired experimental [8–12, 16–20, 37–43] and theoretical [14, 44–51] studies on the structural, bonding, elastic and electronic properties of these materials.

The aim of this study was to predict new, currently unknown superconducting materials within the M2AX family. To benchmark the approach, superconducting properties of four hexagonal ternary carbides Nb2AC (A: S, Ge, As and Sn) were studied and compared against known experimental data, to create a high-throughput screening approach which enabled a larger set of materials to be tested. The most promising candidate identified was then studied in more detail.

In 1999, Nb2SnC was discovered to exhibit superconductivity at 5 K [28]. Ab initio calculations of the structural properties of Nb2SC [46] were first performed in 2006. In the same year, the structural and electronic properties of Nb2SnC and Nb2SC1−x were investigated [52]. In addition, Nasir et al have studied the structural parameters, elastic, electronic, thermodynamic and optical properties of Nb2AC (A: S and Sn) [53]. The other four materials, Nb2AC (A: Al, Ge, As and Sn), have also been synthesized [54, 55] and variety of experimental and theoretical studies have revealed the structural [56–66], electronic [57–73], mechanical and vibrational [64–73], thermodynamic [56, 63], thermal [63–65, 70, 74], magnetic [74], transport [74] and optical [63–65] properties. In 2005, Hettinger et al [10] analysed the electronic, magnetoresistance, thermoelectric, thermal and elastic properties of Nb2AlC and evaluated resistivity as a function of temperature in the 5 to 300 K temperature regime. The aim of that study was not to study superconductivity, and so they did not explore the low temperature range in any detail, with only 1 data point below 15 K. Consequently, they did not find any strong evidence of superconductivity in this material and although in 2009 the same group [75] reported a superconducting transition temperature of 440 mK with electrical transport measurements, this was for a thin film with a different stoichiometry and hence not a bulk M2AX phase. Using density functional theory (DFT), Hadi et al have calculated the electronic structure, bonding natures and defect processes of Nb2SnC which demonstrated that the Nb–C bond is stronger than the covalent Nb–Sn bond [57]. In addition, Bouhemadou et al published ab initio calculations of the structural, electronic and elastic properties of Nb2GeC [69] and shown that the key component of the bonding is hybridizations of Nb(d)–C(p) and Nb(d)–Ge(p). An experimental study [29] of the electronic resistivity, magnetoresistance and heat capacity of Nb2AsC showed that the electron–phonon coupling parameter λ ∼ 0.340 for this superconductor and hence they predicted a superconducting temperature Tc ∼ 2 K. Nasir et al have also theoretically estimated the electron–phonon coupling constants for Nb2SC and Nb2SnC to be λ ∼ 0.49 and ∼ 0.59, respectively [53] using a Debye temperature approach. Finally, Zhao et al have calculated the interaction of Nb2SnC with Li ions which may be promising for energy storage due to the presence of Sn layers [43].

While structural, electronic, elastic, thermodynamic and vibrational properties of Nb2AC (A: Al, S, Ge, As and Sn) have been studied extensively by theoretical and experimental means, to the best of our knowledge a detailed theoretical investigation of the electron–phonon coupling in these materials is still missing from the literature. A study of the electron–phonon interaction is essential to understand the origin of superconductivity in these materials (within the realm of the conventional Bardeen–Cooper–Schrieffer (BCS) theory [76]). Hence, this work presents an ab initio study, using the plane-wave pseudopotential approach to DFT, of the structural, electronic and phonon properties, the Fermi surface and the electron–phonon interaction. The linear response theory [77, 78] and the Migdal–Eliashberg theory [79, 80] are combined to determine the Eliashberg spectral function of Nb2AC (A: S, Ge, As and Sn). These quantities are then used to study the source of superconductivity in these materials and the effect of changing the transition metal atom at the A-site on the superconducting properties and the transition temperatures Tc.

For the four materials which were known to be superconducting, Nb2AC (A: S, Ge, As and Sn) the Eliashberg spectral function αF(ω), the electron–phonon coupling parameter λ, and the logarithmic average of phonon frequency ωln were calculated and used to compute the superconducting transition temperatures Tc. These were then analysed in terms of the Fröhlich model [76] and compared with the corresponding experimental values of Tc. This showed that the Fröhlich model worked well for this class of materials and so was used as the basis for a screening approach to study more Nb–C M2AX phases for which there are no known previous superconductivity studies. The density of states (DOS) at the Fermi level (N(EF)) for Nb2AC with different choices for A element (Zn, Cd, Al, Ga, In, Ti, Si, Pb and P) were calculated and used as an input to the Fröhlich model, which showed that Nb2AlC was likely to have the highest Tc of this set. Finally, the full electron-coupling constant calculations using the Migdal–Eliashberg theory were performed for Nb2AlC to
produce a more robust prediction for \( T_c \). The value of \( T_c \) found using this approach and the Allen–Dynes formula is remarkably close to the prediction from our simple Fröhlich model.

We have also studied the electronic properties of Nb₂AC (A: Al, S, Ge, As and Sn). Recently, it has been realized that symmetry plays a key role in topological phases [81–83]. Metals can be classified from topological points as trivial metals (Ms) and non-trivial topological metals (TMs). Three-dimensional topological insulators are described by a spin-helical Dirac cone [81–83]. Compared to other topological superconductors [84–87], our electronic results suggest that Nb₂AC (A: Al, S, Ge, As and Sn) might be topological superconductors, and this would make an interesting topic for further study.

2. Method

This study used the Quantum ESPRESSO (QE) ab initio simulation package [77, 78, 88] which is based upon the plane-wave pseudopotential approach to DFT [89]. The exchange-correlation functional is approximated using the Perdew–Burke–Ernzerhof (PBE) scheme [90] and ultrasoft pseudopotentials [91] are used throughout. The plane-wave basis cut-off is taken as 60 Ry for all calculations. The Kohn–Sham equations were solved using an iterative conjugate gradient scheme.

The Brillouin zone integration for the computation of total energies of Nb₂AC (A: Al, S, Ge, As and Sn) used the Monkhorst–Pack sampling scheme [92] with a\((36 \times 36 \times 8)\) grid of \( k \)-points (maximum spacing of \( 0.01 \times 2\pi \text{ Å}^{-1} \)). Structure optimisation was performed using the total energy minimisation and zero atomic force criteria. Additional electronic band structure and DOS calculations were performed using a denser \((40 \times 40 \times 10)\) \( k \)-point grid.

Phonon calculations for each structure were performed within the harmonic approximation using the linear response approach [77, 78, 88] in QE with a \((4 \times 4 \times 4)\) \( q \)-point grid to sample the Brillouin zone. The dynamical matrices were calculated on a \( 4 \times 4 \times 4 \) grid and Fourier interpolation [93] was used to calculate phonons for any chosen \( q \)-point. The linear-response approach and the Migdal–Eliashberg theory [79, 80] are combined to compute the electron–phonon matrix elements and from this, a value for the superconducting transition temperature \( T_c \) within BCS theory.

The full calculation of \( T_c \) using Migdal–Eliashberg theory is computationally expensive and typically takes several weeks per material. This is therefore unsuitable for a high throughputs screening approach to identifying new candidate superconductors. Given the structural and electronic similarity of the hexagonal ternary carbides considered, it may seem that the effect of changing the \( A \) element in Nb₂AC is akin to the superconducting isotope effect. This was discovered experimentally in Hg by Maxwell and Reynolds [94, 95] and explained theoretically by Fröhlich [96]. The Fröhlich model has \( T_c \sim M^{-p} \), where \( M \) is the isotope mass and \( p \) is the isotope coefficient, and it is often presumed \( p = 1/2 \). In this work, the Fröhlich model is used as the basis for a high throughputs screening approach to study more Nb–C \( M_2AX \) phases, with

\[
T_c \sim \frac{N(E_F)}{\sqrt{M}},
\]

where \( M \) is the mass of a formula unit. The calculation of \( N(E_F) \) is much faster than the electron–phonon matrix elements (typically only a few minutes) and this can be used with the observed trend in \( T_c \) vs \( N(E_F)/\sqrt{M} \) for known Nb₂AC materials to predict the superconducting transition temperatures of candidate materials for which there are no known previous superconductivity studies. The most promising of these is found to be Nb₂AlC and so this was then studied in more detail using the Migdal–Eliashberg theory, which confirmed the prediction of \( T_c \).

3. Results

3.1. Structural and electronic properties

The \( M_2AX \) phases studied, Nb₂AC (A: S, Ge, As and Sn) all crystallize in the hexagonal structure with space group \( P6_3/mmc \). The primitive unit cell includes two formula unit (eight atoms), with occupied Wyckoff positions \( 4f (1/3, 2/3, z) \) for Nb, \( 2d (1/3, 2/3, 3/4) \) for \( A \) (A: S, Ge, As and Sn) and \( 2a (0, 0, 0) \) for C atoms, where \( z \) is the internal free coordinate. Hence, the structure is defined by two lattice parameters, \( a \) and \( c \), and one internal structural parameter, \( z \). Figure 1 shows the atomic arrangement in the hexagonal unit cell of Nb₂AC (A: S, Ge, As and Sn), where blocks of Nb-carbides [NbC] (formed by edge-shared Nb₆C octahedra) are sandwiched between A atomic sheets.

Each compound was structure optimized and then the Murnaghan equation of state was used to obtain the crystal total energy versus cell volume in order to calculate lattice constants (\( a \) and \( c \)), and the optimised internal parameter (\( z \)). The determined equilibrium lattice constants (\( a \) and \( c \)), the internal parameter (\( z \), the
Figure 1. The hexagonal crystal structure of Nb$_2$AC ($A$: Al, S, Ge, As and Sn), where blocks of Nb-carbides [NbC] (formed by edge-shared Nb₆C octahedra) are sandwiched with $A$ atomic sheets.

closest Nb–Nb ($d_{Nb-Nb}$), Nb–$A$ ($d_{Nb-A}$) Nb–C ($d_{Nb-C}$) distance, bulk modulus ($B$) and its pressure derivative $B'$, and the comparison with available experimental and theoretical results are presented in table 1. The lattice parameters obtained are in good agreement with the previous experimental and theoretical results [7, 12, 28, 97]. In particular, each lattice parameter differs from its experimental value by less than 2%, whereas the calculated values of the internal coordinate for Nb$_2$AC ($A$: S, Ge, As and Sn) are almost equal to the corresponding experimental value [12, 28, 52, 73].

Table 1 also contains results for relaxed bond lengths of Nb$_2$AC, where $d_{Nb-Nb}$, $d_{Nb-A}$ and $d_{Nb-C}$ indicate the bonding between transition metal (Nb) atoms, Nb and $A$ group atoms, and transition metal and C, respectively. The Nb–Nb distances in the different materials are all longer than in elemental Nb (2.86 Å). The bond length between Nb and C atoms in each of the materials is smaller than the sum of the covalent radii of Nb (1.98 Å) and C (0.67 Å), which implies that the Nb–C bond has both ionic and covalent character, and in particular, the covalent interaction for Nb–C is strongest in the Nb$_2$SC material. The Nb–$A$ distances are all longer than the corresponding Nb–C distances for each material, and so the Nb–C bond is much stronger and more covalent than Nb–$A$ (where $A$ = S, Ge, As and Sn).

The electronic band structure along high symmetry paths in the Brillouin zone of hexagonal Nb$_2$AC ($A$: S, Ge, As and Sn) is shown in figure 2(a) with the Fermi level set to 0 eV. The DOS at the Fermi level ($N(E_F)$) is a key quantity for metallic phases and in the calculation of superconductivity. The corresponding total DOS and the partial density of states (PDOS) of each constituent, broken into site and angular momentum contributions, are illustrated in figure 2(b). The calculated electronic structure explicitly shows the metallic feature of all the studied materials, since some of the bands (mainly the Nb 4d states) cross the Fermi level. The electronic band structure agrees very well with previous work [53, 62, 73]. Note that the number of valence bands crossing the Fermi level is 6 in Nb$_2$SC while it is 4 in the other three superconductors. Hence, it may be expected that Nb$_2$SC will have a higher transition temperature than the materials considered, but qualitatively, the electronic band structures shown in figure 2 are all very similar to each other.

The valence DOS of Nb$_2$SC, Nb$_2$GeC, Nb$_2$AsC and Nb$_2$SnC is separated into two regions by a gap of 3.1, 0.5, 3.2 and 0.2 eV respectively. From figure 2(b), the DOS of Nb$_2$SnC is broadly similar to Nb$_2$GeC, which is not surprising since Sn and Ge are isoelectronic in pseudopotential calculations, while Nb$_2$SC and Nb$_2$AsC, are more different.

Analysis of the PDOS of Nb$_2$SnC shows that the lowest energy region, $-12.1 < E < -10.7$ eV is dominated by the C 2s states with appreciable contributions from the Nb 5p and 4d states. The next region, $-10.5 < E < -6.1$ eV is also characterized by Sn 5s states with C 2p and Nb 4d states. The main valence band region ranging from $-6.1 < E < -3.8$ eV comprises hybridized Nb 4d and C 2p states, indicating covalent Nb–C bonding. The region $-3.8 < E < E_F$ eV originates from Nb 4d states with some weak hybridization of Nb 4d and Sn 5p states in the range $-3.6 < E < -1.5$ eV which is in agreement with the long distance of Nb–Sn bond as discussed previously. Finally, electronic states close to the Fermi level must be analysed in more detail, since Cooper pairs in the BCS theory are made from electrons possessing energies close to the Fermi level. The DOS at the Fermi level $N(E_F) = 3.843$ states/eV with contributions from Nb, Sn and C atoms of
## Table 1. Structural properties of the hexagonal Nb$_2$AC ($A$: S, Ge, As and Sn) for this work in bold, and their comparison with previous experimental and theoretical results.

| Source      | $a$ (Å) | $c$ (Å) | $d_{3\overline{1}0-\overline{1}0}$ (Å) | $d_{3\overline{0}-\overline{0}}$ (Å) | $d_{3\overline{0}-\overline{C}}$ (Å) | $B$ (GPa) | $B'$ |
|-------------|---------|---------|---------------------------------|---------------------------------|---------------------------------|-----------|-----|
| Nb$_2$SC    | 3.305   | 11.651  | 0.095  | 2.926  | 2.625  | 2.207  | 197 | 4.85 |
| Exp [28]    | 3.294   | 11.533  | 0.096  | 2.601  | 2.204  |          |     |      |
| Exp [60]    | 3.294   | 11.784  |        |        |        |          |     |      |
| GGA [42]    | 3.278   | 11.491  | 194    |        |        |          |     |      |
| GGA [46]    | 3.298   | 11.731  | 220    |        |        |          |     |      |
| GGA [48]    | 3.320   | 11.799  | 0.095  | 2.215  | 2.215  |          |     |      |
| GGA [52]    | 3.294   | 11.784  | 0.096  | 2.601  | 2.204  |          |     |      |
| GGA [53]    | 3.290   | 11.670  | 0.096  | 2.933  | 2.620  | 3.483  | 197 |      |
| GGA [66]    | 3.307   | 11.642  | 0.095  | 2.204  | 2.204  |          |     |      |
| GGA [73]    | 3.301   | 11.647  | 0.095  | 2.204  | 2.204  |          |     |      |
| Nb$_2$GeC   | 3.244   | 12.667  | 0.092  | 2.995  | 2.739  | 2.208  | 197 | 4.85 |
| Exp [12]    | 3.240   | 12.820  |        |        |        |          |     |      |
| Exp [20]    | 3.255   | 12.565  |        |        |        |          |     |      |
| Exp [36]    | 3.250   | 12.540  |        |        |        |          |     |      |
| GGA [12]    | 3.265   | 12.653  | 0.093  |        |        |          | 192 |      |
| GGA [49]    | 3.227   | 13.068  | 2.991  | 2.778  | 2.214  |          |     |      |
| GGA [56]    | 3.236   | 12.684  | 0.092  | 2.995  | 2.204  |          |     |      |
| GGA [62]    | 3.254   | 12.590  | 0.092  |        |        |          | 233 |      |
| GGA [97]    | 3.259   | 12.600  | 1.166  | 1.985  | 192    |          |     |      |
| LDA [69]    | 3.237   | 12.358  | 0.095  |        |        |          | 207 | 4.35 |
| Nb$_2$AsC   | 3.331   | 12.018  | 0.094  | 2.967  | 2.685  | 2.231  | 208 | 4.53 |
| Exp [7]     | 3.310   | 11.900  |        |        |        |          |     |      |
| Exp [15]    | 3.327   | 11.917  |        |        |        |          | 224 | 4.00 |
| GGA [48]    | 3.344   | 12.048  | 0.094  |        |        |          | 234 |      |
| GGA [63]    | 3.324   | 11.979  | 0.095  | 3.73   | 2.230  |          |     |      |
| GGA [73]    | 3.323   | 11.995  | 0.095  | 2.969  | 2.675  | 2.228  | 206 |      |
| GGA [97]    | 3.339   | 12.000  | 1.129  | 1.870  | 204    |          |     |      |
| GGA [101]   | 3.355   | 12.075  |        |        |        |          |     |      |
| LDA [61]    | 3.317   | 11.900  | 0.094  | 2.950  | 2.360  | 2.220  |     |      |
| Nb$_2$SnC   | 3.257   | 14.027  | 0.082  | 2.987  | 3.002  | 2.208  | 170 | 4.88 |
| Exp [7]     | 3.241   | 13.802  |        |        |        |          |     |      |
| Exp [13]    | 3.240   | 13.802  | 2.963  | 2.193  |        |          |     |      |
| Exp [30]    | 3.220   | 13.707  |        |        |        |          |     |      |
| Exp [60]    | 3.775   | 15.527  |        |        |        |          |     |      |
| GGA [48]    | 3.277   | 13.903  | 0.083  |        |        |          | 171 |      |
| GGA [52]    | 3.252   | 13.844  | 0.083  | 2.969  | 2.986  | 2.208  |     |      |
| GGA [53]    | 3.260   | 13.910  | 0.082  | 2.957  | 3.001  | 2.201  | 163 |      |
| GGA [57]    | 3.263   | 13.906  | 0.082  |        |        |          | 171 |      |
| GGA [65]    | 3.258   | 13.918  | 0.082  |        |        |          | 160 |      |
| GGA [73]    | 3.259   | 13.910  | 0.082  | 2.961  | 2.998  | 2.201  | 166 |      |
| GGA [97]    | 3.273   | 13.850  | 1.141  | 2.321  |        |          | 162 |      |
| GGA [107]   | 3.244   | 13.754  | 0.083  |        |        |          | 206 |      |
| GGA [108]   | 3.178   | 13.775  | 0.083  |        |        |          | 161 |      |
| LDA [71]    | 3.201   | 13.535  | 0.085  |        |        |          | 188 | 4.48 |

approximately 88%, 9% and 3% respectively. Hence the conduction properties are dominated by the Nb 4d electrons.

Repeating this analysis for the electronic DOS of the three other materials Nb$_2$AC ($A$: S, Ge and As) shows a very similar pattern, with hybridization between Nb–C and Nb–$A$ atoms and similar values of $N(E_F)$: 3.452 states/eV for Nb$_2$SC, 3.992 states/eV for Nb$_2$GeC and 3.005 states/eV for Nb$_2$AsC. These results are consistent with previous theoretical studies [29, 53, 62]. As expected, $N(E_F)$ for Nb$_2$GeC and Nb$_2$SnC are very similar, as these are isoelectronic as noted before, while there is a bigger difference with the other two materials.

The impact of $N(E_F)$ on superconductivity can be estimated from the McMillan–Hopfield expression [98] for the electron–phonon coupling parameter

$$\lambda = \frac{N(E_F) \langle F^2 \rangle}{M \omega^2},$$

where $\langle F^2 \rangle$ is the average squared phonon frequency, $\langle F^2 \rangle$ is the average squared electron–phonon matrix element and $M$ is the mass. This shows $\lambda \propto N(E_F)$ and so as the calculated value $N(E_F)$ of Nb$_2$GeC is higher than the other materials, it should lead to an increase in the value of $T_c$ if all other effects are similar.
Figure 2. (a) The electronic band structure for the hexagonal phase of Nb₂AC (A: S, Ge, As and Sn). The Fermi energy corresponds to 0 eV. (b) The total and atomic projected electronic local DOS for the hexagonal phase of Nb₂AC (A: S, Ge, As and Sn).

The Fermi surface of Nb₂AC (A: S, Ge, As and Sn) is formed mainly by the Nb 4d-like bands, which are responsible for the electrical conductivity. Further insight into the $E_F$ crossed bands behaviour is gained from visualization of the Fermi surface of these materials, as in figure 3, which shows good agreement with previous studies [56, 57, 64, 73]. In general, these show both electron and hole-like sheets. Along the $\Gamma$–A direction, the Fermi surface is completely prismatic and cylindrical and shows electron-like behaviour, while hole-like
sheets occur at the corners of the Brillouin zone along the $H–K$ and $L–M$ directions. The $\text{Nb}_2\text{A}_\text{C}(\text{A}: \text{S, Ge, As and Sn})$ compounds have four Fermi surface sheets. The Fermi surface of $\text{Nb}_2\text{SC}$ material is electron-like sheets of hexagonal cross-section topology along the $\Gamma–A$ directions and wing sheets along the $L–M$ and $H–K$ direction. Fermi nesting may play an important role in enhancing electron–phonon interactions [99, 100] and hence boosting superconductivity. A detail examination of the Fermi nesting in $\text{Nb}_2\text{GeC}$ is given in the supplementary material (https://stacks.iop.org/EST/3/045001/mmedia). The calculated Fermi surface of $\text{Nb}_2\text{GeC}$ is in excellent agreement with previously published Fermi surface results [48, 56]. In addition, the Fermi surface of $\text{Nb}_2\text{SnC}$ compound is very similar to that of $\text{Nb}_2\text{GeC}$. Finally, the first sheet of $\text{Nb}_2\text{AsC}$ has complex nesting properties that suggest both hole and electron pocket features.

### 3.2. Phonons and electron–phonon interaction

The primitive unit cell of all the materials investigated contain 8 atoms and so there are 24 phonon branches for any wave vector, of which three are acoustic and the rest are optical phonon branches. The zone centre optical phonon modes can be categorized according to their reducible representation of the point group $\text{D}_{6h}$ (6/mmm).

From group theory, the symmetries of the optical zone-centre phonon modes are:

$$
\Gamma = A_{1g} + 2A_{2u} + 2B_{1g} + 2B_{2u} + E_{1g} + 2E_{3g} + 2E_{1u} + 2E_{2u},
$$

where $A_{1g}$, $E_{1g}$ and $E_{2g}$ are Raman active (R) modes while $A_{2u}$ and $E_{1u}$ are IR-active (IR) modes. The rest of the optical modes are silent, as the one-dimensional $A$ and $B$ modes involve displacements along the $z$ direction and the doubly degenerate $E$ modes represent displacement in the $x–y$ plane. A comparison of the zone-centre phonon frequencies and the electron–phonon coupling parameters for $\text{Nb}_2\text{AC}(\text{A}: \text{S, Ge, As and Sn})$ is presented in table 2. This shows that the electron–phonon coupling parameters of the $A_{1g}$ phonon mode is considerably larger than the corresponding values for the remaining phonon modes. Calculated Raman active and IR-active phonon frequencies are in acceptable agreement with previously published phonon results [73, 101].

Phonons have a crucial role in the BCS superconductivity of these materials, and so the calculated phonon dispersion relations for $\text{Nb}_2\text{SC}$, $\text{Nb}_2\text{GeC}$, $\text{Nb}_2\text{AsC}$ and $\text{Nb}_2\text{SnC}$ are shown in figures 4(a)–(d), respectively. The phonon calculations show that each of the $\text{Nb}_2\text{AC}(\text{A}: \text{S, Ge, As and Sn})$ compounds are dynamically stable.
Table 2. The calculated zone-centre optical phonon frequencies ($\nu$ in THz) and their electron–phonon coupling parameters ($\lambda$) for hexagonal Nb$_2$AC (A: S, Ge, As and Sn) and their comparison with available previous experimental and theoretical results. IR and R indicate infrared-active and Raman-active vibrations, respectively.

| Material  | $E_{2u}$ | $B_{2u}$ | $E_{1g}$ (R) | $E_{1g}$ (IR) | $B_{1g}$ | $A_{2u}$ (IR) | $E_{2g}$ (R) | $A_{1g}$ (R) | $B_{1g}$ | $B_{2g}$ | $A_{2u}$ (IR) | $E_{2u}$ | $E_{1u}$ (IR) |
|-----------|----------|----------|--------------|--------------|----------|---------------|--------------|--------------|----------|----------|---------------|----------|--------------|
| Nb$_2$SC ($\nu$) | 2.611 | 4.070 | 4.897 | 5.739 | 6.801 | 7.379 | 7.871 | 7.917 | 9.806 | 14.918 | 15.159 | 19.229 | 19.289 |
| Nb$_2$SC ($\lambda$) | 0.016 | 0.037 | 0.043 | 0.046 | 0.036 | 0.023 | 0.012 | 0.061 | 0.105 | 0.029 | 0.012 | 0.003 | 0.004 | 0.006 |
| GGA [73]($\nu$) | 4.224 | 5.546 | 4.869 | 7.105 | 5.905 | 7.324 | 15.074 | 18.767 |
| Nb$_2$GeC ($\nu$) | 2.937 | 3.759 | 3.421 | 5.882 | 5.609 | 7.821 | 4.559 | 5.902 | 7.444 | 8.875 | 17.273 | 17.221 | 18.409 | 18.338 |
| Nb$_2$GeC ($\lambda$) | 0.000 | 0.175 | 0.076 | 0.736 | 0.097 | 0.000 | 0.009 | 0.958 | 1.516 | 0.163 | 0.005 | 0.000 | 0.001 | 0.011 |
| Nb$_2$AsC ($\nu$) | 3.261 | 4.414 | 3.855 | 5.738 | 5.612 | 7.478 | 5.918 | 6.680 | 8.280 | 8.306 | 15.880 | 15.840 | 18.001 | 17.676 |
| Nb$_2$AsC ($\lambda$) | 0.011 | 0.029 | 0.009 | 0.065 | 0.016 | 0.003 | 0.003 | 0.062 | 0.066 | 0.042 | 0.009 | 0.001 | 0.002 | 0.007 |
| Exp [101]($\nu$) | 4.077 | 6.145 | 4.077 | 6.145 | 6.664 | 6.608 | 7.468 | 8.328 | 14.501 | 17.499 |
| GGA [73]($\nu$) | 4.970 | 6.497 | 6.664 | 6.608 | 7.468 | 8.328 | 14.501 | 17.499 |
| GGA [101]($\nu$) | 3.897 | 5.905 | 6.695 | 8.364 | 14.501 | 17.499 |
| Nb$_2$SnC ($\nu$) | 2.140 | 3.331 | 2.251 | 5.607 | 4.101 | 5.788 | 2.916 | 5.279 | 7.571 | 7.637 | 16.253 | 16.288 | 18.499 | 18.354 |
| Nb$_2$SnC ($\lambda$) | 0.000 | 0.114 | 0.199 | 0.342 | 0.034 | 0.000 | 0.024 | 0.544 | 1.999 | 0.116 | 0.005 | 0.000 | 0.000 | 0.018 |
| GGA [73]($\nu$) | 2.698 | 7.543 | 7.084 | 4.701 | 7.129 | 7.150 | 15.344 | 17.448 |
as there are no negative frequencies observed. However, the different A atoms cause significant changes in the features of the dispersion curves.

It can be seen that the phonon spectra of Nb$_2$AC (A: S, Ge, As and Sn) separates into two distinct regions, with a low-frequency region up to 11 THz which contains fifteen optical and three acoustic phonon modes,
Figure 5. The calculated electron–phonon spectral function $\alpha^2 F(\omega)$ (red line) and the variation of the electron–phonon coupling parameter (blue line) with rising frequency $\lambda(\omega)$ of (a) Nb$_2$SC (b) Nb$_2$GeC (c) Nb$_2$AsC and (d) Nb$_2$SnC.

and a high-frequency region from 15 THz to 20 THz which contains six optical modes. These two regions are separated from each other by a significant gap. It should be noted that the $E_{2g}$ branch of Nb$_2$GeC has a phonon anomaly which has been observed along the $\Gamma$–$K$ and $M$–$\Gamma$ direction. Also, the lower doubly degenerate vibrational branch shows anomaly along the $A$–$H$ direction. A more detailed study of the softening of these modes in selected directions is given in the supplementary material.

To understand the contributions of various phonon modes in the phonon spectrum, the results of total and partial vibrational density of states (VDOS) for these materials, Nb$_2$AC ($A$: S, Ge, As and Sn), are illustrated in figures 4(e)–(h), respectively. In the low-frequency region up to 11 THz, there is significant overlap and hybridization of Nb–$A$ modes, for Nb$_2$AC ($A$: Ge, As and Sn), whereas the hybridization is lost for Nb$_2$SC. In addition, when $A = S$ there is a region around 10 THz which is a near pure $A$-atom mode, and more significantly, for $A = Sn$ the very lowest frequency region up to 3 THz is dominated by a near pure Sn-atom mode. In the high-frequency region from 15 THz to 20 THz, the VDOS is mainly characterised by the motions of C atoms as expected due to their light mass.

The electron–phonon interaction has been investigated with the linear response theory [77, 78] approach to the Migdal–Eliashberg theory [79, 80]. The scattering of an electron in state $|k\nu\rangle$ to state $|k + \mathbf{q}m\rangle$ due to the phonon mode $\omega_{\mathbf{q}j}$ perturbation is given by the electron–phonon matrix elements $\delta_{k+\mathbf{q}m;k\nu}$ which have been estimated self-consistently by the linear response theory [77, 78]. From these matrix elements, the phonon linewidth $\gamma_{\mathbf{q}j}$ is given as

$$\gamma_{\mathbf{q}j} = 2\pi\omega_{\mathbf{q}j}\sum_{k\nu\nu'}|\delta_{k+\mathbf{q}m;k\nu}|^2\delta(\varepsilon_{k\nu} - \varepsilon_F)\delta(\varepsilon_{(k+\mathbf{q})m} - \varepsilon_F).$$

(4)

The electronic DOS, phonon modes and linewidths can be used to calculate the Eliashberg spectral function $\alpha^2 F(\omega)$ from

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(E_F)}\sum_{\mathbf{q}j}\gamma_{\mathbf{q}j}\delta(\omega - \omega_{\mathbf{q}j}),$$

(5)

where $N(E_F)$ refers to the electronic DOS at the Fermi level. The Eliashberg spectral function $\alpha^2 F(\omega)$ can be used to calculate the average electron–phonon coupling constant

$$\lambda(\omega) = 2\int \frac{\alpha^2 F(\omega)}{\omega} d\omega.$$  

(6)
Table 3. DOS at the Fermi level \(N(E_F)\), logarithmic frequency \(\omega_{ln}\), the average electron–phonon coupling parameter \(\lambda\) and the superconducting transition temperature \(T_c\) in K for the hexagonal Nb_2AC \((A: S, Ge, As and Sn)\) for this work in bold, and their comparison with available previous experimental and theoretical results.

| Material    | \(N(E_F)\) (states/eV) | \(\omega_{ln}\) (K) | \(\lambda\) | \(T_c\) (K) |
|-------------|-------------------------|----------------------|-------------|-------------|
| Nb_2SC      | 3.452                   | 249.124              | 0.739       | 7.720       |
| Exp [28]    |                         |                      |             |             |
| Exp [60]    |                         |                      |             |             |
| GGA [42]    |                         |                      |             |             |
| GGA [52]    | 3.036                   |                      |             |             |
| GGA [53]    | 3.540                   |                      | 0.490       |             |
| GGA [66]    | 3.290                   |                      |             |             |
| GGA [73]    | 3.580                   |                      |             |             |
| Nb_2GeC     | 3.992                   | 298.347              | 0.685       | 9.830       |
| Exp [36]    |                         |                      |             |             |
| GGA [62]    |                         |                      |             |             |
| Nb_2AsC     | 3.005                   | 300.906              | 0.440       | 2.094       |
| Exp [29]    | 3.000                   |                      | 0.340       | 2.000       |
| GGA [61]    | 3.000                   |                      | 0.400       |             |
| GGA [73]    | 3.010                   |                      |             |             |
| Nb_2SnC     | 3.843                   | 258.140              | 0.614       | 6.314       |
| Exp [29]    |                         | 0.220                |             |             |
| Exp [30]    |                         |                      |             |             |
| Exp [60]    |                         |                      |             |             |
| GGA [52]    | 3.556                   |                      | 0.590       |             |
| GGA [53]    | 3.820                   |                      |             |             |
| GGA [57]    | 3.620                   |                      |             |             |
| GGA [65]    | 3.440                   |                      |             |             |
| GGA [67]    | 3.720                   |                      |             |             |
| GGA [73]    | 3.680                   |                      |             |             |
| GGA [107]   | 3.710                   |                      |             |             |

From figure 5, it is apparent that \(\lambda(\omega)\) is dominated by the contribution from the lowest frequency region, where \(\lambda \propto \omega\). In particular, in Nb_2AC \((A: S, Ge, As and Sn)\), the proportional contribution to \(\lambda = 92\%, 84\%, 87\% \) and \(88\%\) and is dominated by the coupled motion of Nb and A atoms while \(N(E_F)\) is dominated by the Nb 4d states. This contribution is largest for Nb_2SC because of the lack of Nb–S hybridization seen in the phonon VDOS (figure 4(e)). The high-frequency region makes only a minor contribution to \(\lambda = 8\%, 16\%, 13\% \) and \(12\%\) respectively, which is expected as this region is dominated by the light C atom phonon modes, and from figure 2 it is apparent that \(N(E_F)\) is dominated by Nb 4d-states with very little contribution from C.

The value of \(\lambda(\omega)\) can then be used to compute the logarithmic average phonon frequency \(\omega_{ln}\) using

\[
\omega_{ln} = \exp \left( 2\lambda^{-1} \int_0^{\infty} \frac{d\omega}{\omega} \alpha^2 F(\omega) \ln \omega \right)
\]

resulting in \(\omega_{ln} = 249.124\ K, 298.347\ K, 300.906\ K \) and \(258.140\ K\) for Nb_2AC \((A: S, Ge, As and Sn)\), respectively.

Finally, these values of \(\lambda\) and \(\omega_{ln}\) are used to calculate the superconducting transition temperature \(T_c\) using the Allen–Dynes modification of the McMillan formula:

\[
T_c = \frac{\omega_{ln}}{1.2} \exp \left( -\frac{1.04(1 + \lambda)}{\lambda - \mu^* (1 + 0.62\lambda)} \right)
\]

where \(\mu^*\) represents an effective screened Coulomb repulsion parameter. In most studies, the value of the \(\mu^*\) varies between 0.10 and 0.16 [102, 103].

Here, the Coulomb repulsion parameter is chosen to be \(\mu^* = 0.10\), which results in \(T_c \approx 7.720\ K, 9.830\ K, 2.094\ K \) and \(6.314\ K\) for Nb_2Ac \((A: S, Ge, As and Sn)\), respectively, which agree very well with the experimental values, justifying the choice of \(\mu^*\). The value of \(T_c\) obtained is in good agreement with the known experimental value for all materials as can be seen in table 3. Note that the experimental data of Lofland et al for Nb_2AsC suggested a superconducting transition temperature of 10 K based upon the resistivity measurements, but 2 K on the basis of the magnetic susceptibility. They suggested that there may be a superconducting transition near to 2 K, which is supported by the theoretical calculations in this work. To demonstrate the sensitivity of \(T_c\) to \(\mu^*\), the average \(T_c\) value using different Coulomb repulsion parameters (between 0.10 and 0.16) was also calculated, and found to be 6.748 K, 8.625 K, 1.557 K and 5.392 K for Nb_2Ac \((A: S, Ge, As and Sn)\), respectively.
3.3. Fröhlich model

The Fröhlich model is used as the basis for the analysis in figure 6, which shows there is a linear relationship between the critical temperature \( T_c \) and \( N(E_F)/\sqrt{M} \) value. The \( T_c \) value of the four superconductors (Nb\(_2\)SC, Nb\(_2\)GeC, Nb\(_2\)AsC and Nb\(_2\)SnC) calculated using the Eliashberg theory (with \( \mu^* = 0.10 \)) are plotted with black circles in figure 6(a) with the corresponding experimental \( T_c \) values shown in red with a worst-case error in \( T_c \) of \( \sim 2 \) K. A linear regression to the theoretical results is shown as a black line. According to our Fröhlich model predictions and Eliashberg theory calculations, the calculated \( T_c \) values for Nb\(_2\)SC and Nb\(_2\)SnC were found to be slightly different (1–2 K) from the experimental values. This may be due to the lack of Nb modes in the lowest-frequency region, with the lighter mass of S than Nb resulting in an overestimate of \( T_c \) and the heavier mass of Sn resulting in an underestimate of \( T_c \).

It is proposed that this linear trend will hold for all Nb\(_2\)AC materials and hence this model be used as the basis for a high-throughput screening approach to rapidly evaluate similar materials for which \( T_c \) is not known. This is very useful, as it is much faster to perform an electronic DOS (\( \sim 1 \) h) than to calculate the full electron–phonon coupling (\( \sim 300 \) h). This approach was then used to study the structural and electronic properties of Nb\(_2\)AC (where \( A: \) Zn, Cd, Al, Ga, In, Ti, Si, Pb and P) materials within the \( M_2AX \) family, for
which there have been no known studies of superconductivity. The calculation of $N(E_F)$ for Nb$_2$AC (where A: Zn, Cd, Al, Ga, In, Tl, Si, Pb and P) is much faster than the detailed phonon-based approach, and is shown as the blue dashed lines in figure 6(b). This predicts that Nb$_2$AC would have the highest $T_c$ of the unknown materials with an estimated $T_c \sim 7$ K. There is very little experimental data on the low-temperature properties of Nb$_2$AC. This work predicts that this material should be a superconductor with a transition temperature around 7 K and this should be apparent in magnetic susceptibility measurements. To test this prediction, the detailed properties of Nb$_2$AC including the electron–phonon coupling are calculated and presented in the following section.

3.4. Electronic, phonons and electron–phonon interaction properties of Nb$_2$AC

As before, geometry optimization and the Murnaghan equation of state was used to obtain the lattice constants ($a$ and $c$), the internal parameter ($z$), bulk modulus ($B$) and its pressure derivative ($B'$) of Nb$_2$AC. The results are summarized in table 4. The calculated lattice parameters, bulk modulus ($B$), its pressure derivative ($B'$), the closest Nb–Nb ($d_{Nb-Nb}$), Nb–A ($d_{Nb-A}$) and Nb–C ($d_{Nb-C}$) distance are in good agreement with the previous experimental [7, 10, 55] and theoretical results [41, 59, 64, 68, 97, 101, 104]. In addition, the closest bond distances Nb–Nb ($d_{Nb-Nb}$), Nb–A ($d_{Nb-A}$) and Nb–C ($d_{Nb-C}$) distance are calculated, and the bonding properties of Nb$_2$AC are similar to Nb$_2$AC(A: S, Ge, As and Sn) materials, in that the Nb–Nb distance is longer than in elemental Nb (2.86 Å) and the bond length between Nb and C atoms in Nb$_2$AC is smaller than the sum of the covalent radii of Nb (1.98 Å) and C (0.67 Å), which implies that the Nb–C bond has both ionic and covalent character. In particular, the covalent interaction for Nb–C is strongest in the Nb$_2$AC material compared with Nb$_2$AC (A: S, Ge, As and Sn) materials.

The electronic band structure and the corresponding electronic DOS of hexagonal Nb$_2$AC are shown in figures 7(a) and (b), respectively. The calculated electronic structure shows the metallic feature of Nb$_2$AC, since two bands (mainly the Nb 4d states) cross the Fermi level. The electronic band structure coincide very well with previous work [68]. The valence DOS is separated into two regions by a gap of 2.4 eV. The electronic DOS of Nb$_2$AC shows a very similar pattern the other materials (Nb$_2$AC(A: S, Ge, As and Sn)). Analysis of the PDOS of Nb$_2$AC shows hybridization between Nb–C and Nb–Al atoms. In our calculations, $N(E_F)$ is found to be 3.316 states/eV for Nb$_2$AC. The percentage contribution from the Nb site is greater than the other sites, which is very similar to that found in Nb$_2$AC(A: S, Ge, As and Sn).

The Fermi surface of Nb$_2$AC is shown figure 7(c), which is formed mainly by the Nb 4d-like bands. The Nb$_2$AC compound has two Fermi surface sheets, whereas of the other four compounds, Nb$_2$AC (A: S, Ge, As and Sn), contain four sheets. The first sheet of Nb$_2$AC compound is quite complicated, with a central cylindrical part along the $\Gamma$–$A$ direction and wings along the $H$–$K$ directions. The second sheet of Nb$_2$AC is nested with wings along the $L$–$M$ directions.

The zone centre optical phonon modes are summarized in table 5, and are in good agreement with their available experimental [105, 106] and theoretical [64, 101, 105] values. In addition, phonon dispersion relations and VDOS properties of Nb$_2$AC have been calculated and illustrated figures 7(d) and (e), respectively. It can be seen that the phonon spectrum of Nb$_2$AC separates into three apparent regions. In the first region extending up to 8.6 THz, there are thirteen optical and three acoustic phonon modes. The peaks in this first region are dominated by Nb and Al atoms, with hybridization of modes from Nb and Al. The second region (from 9.7 to 10.2 THz) contains two optical branches. These two lower regions are separated from each other by a small gap. In Nb$_2$AC, this second region is dominated by the vibrations of the Al atom. The final region for Nb$_2$AC includes the last six optical phonon modes, separated by a big gap from the second region. In this region, the VDOS is mainly characterised by the motions of C atoms due to their light mass.

### Table 4. Structural properties of Nb$_2$AC for this work in bold, and their comparison with previous experimental and theoretical results.

| Source | $a$ (Å) | $c$ (Å) | $z$ | $d_{Nb-Nb}$ (Å) | $d_{Nb-A}$ (Å) | $d_{Nb-C}$ (Å) | $B$ (GPa) | $B'$ |
|--------|--------|--------|-----|----------------|----------------|---------------|----------|-----|
| Nb$_2$AC | 3.116  | 13.968 | 0.089 | 3.069         | 2.879          | 2.187         | 178      | 4.60|
| Exp [7]  | 3.100  | 13.830 |      |              |                |               |          |     |
| Exp [10] |        |        |      |              |                |               |          |     |
| Exp [35] | 3.106  | 13.888 |      |              |                |               |          |     |
| GGA [41] | 3.127  | 13.896 |      |              |                |               |          |     |
| GGA [59] | 3.119  | 13.920 |      |              |                |               |          |     |
| GGA [64] | 3.122  | 13.926 |      | 3.049        | 2.884          | 2.182         | 175      | 3.90|
| GGA [68] | 3.122  | 13.752 |      |              |                |               |          |     |
| GGA [97] | 3.125  | 13.910 |      |              |                |               |          |     |
| GGA [101] | 3.127  | 13.925 |      |              |                |               |          |     |
| GGA [104] |        |        |      |              |                |               |          |     |
| LDA [64] | 3.082  | 13.703 | 3.017 | 2.835        | 2.157          | 194           |          |     |
Table 5. The calculated zone-centre optical phonon frequencies ($\nu$ in THz) and their electron–phonon coupling parameters ($\lambda$) for hexagonal Nb$_2$AlC and their comparison with available previous experimental and theoretical results. IR and R indicate infrared-active and Raman-active vibrations, respectively.

| Material     | $E_{2u}$ | $B_{2u}$ | $E_{1g}$ (R) | $E_{1g}$ (IR) | $E_{1u}$ (R) | $B_{1g}$ | $A_{1g}$ (IR) | $B_{1u}$ | $A_{2u}$ (IR) | $B_{2u}$ | $A_{2u}$ (IR) | $E_{2u}$ | $E_{1u}$ (IR) |
|--------------|----------|----------|---------------|---------------|---------------|-----------|---------------|-----------|---------------|-----------|---------------|-----------|--------------|
| Nb$_2$AlC ($\nu$) | 2.448    | 3.657    | 4.372         | 5.288         | 5.344         | 5.748     | 6.392         | 7.318     | 9.726         | 10.184    | 18.345        | 18.354    | 18.973       |
| Nb$_2$AlC ($\lambda$) | 0.001    | 0.029    | 0.135         | 0.126         | 0.001         | 0.282     | 0.261         | 0.947     | 0.063         | 0.000     | 0.000         | 0.000     | 0.000        |
| Exp [105]($\nu$) | 4.478    | 4.007    | 4.407         | 5.486         | 5.905         | 6.325     | 7.879         | 17.119    | 17.897        |           |               |           |              |
| Exp [106]($\nu$) | 4.347    | 5.370    | 5.933         | 4.933         | 8.356         | 5.993     | 8.525         | 10.530    | 17.119        |           |               |           |              |
| GGA [64]($\nu$) | 4.317    | 4.786    | 4.317         | 5.786         | 7.525         | 6.325     | 7.879         | 17.119    | 17.897        |           |               |           |              |
| GGA [101]($\nu$) | 4.437    | 5.441    | 4.437         | 5.441         | 8.043         | 5.927     | 8.751         | 10.668    | 19.913        |           |               |           |              |
| LDA [64]($\nu$) | 4.685    | 5.952    | 4.685         | 5.459         | 8.215         | 6.215     | 8.751         | 10.668    | 19.913        |           |               |           |              |
Figure 7. The calculated results of Nb$_2$AlC ((a) electronic band structure, (b) total and atomic projected electronic local DOS (c) Fermi surface (d) phonon dispersion curves (e) total and partial VDOS (f) electron–phonon spectral function $\alpha^2 F(\omega)$ (red line) and the variation of the electron–phonon coupling parameter (blue line)).

The frequency dependence of the Eliashberg spectral function $\alpha^2 F(\omega)$ and the average $\lambda$ value are shown figure 7(f). For Nb$_2$AlC, average $\lambda$ value is found to be 0.646. From figure 7(f), it is apparent that $\lambda$ is dominated by the contribution from the lowest frequency region. The lowest vibrational modes contribute roughly (85\%) to the value of average $\lambda$. The second region only makes a minor contribution to $\lambda = 3\%$. The final contribution to $\lambda$ comes from the highest frequency modes and is a modest proportion of $\lambda = 12\%$. The value of $\lambda$ and $\omega_{ln}$ are summarized in table 6 and used in the Allen–Dynes modified McMillan formula, with $\mu^* = 0.10$, to calculate $T_c \sim 6.709$ K for Nb$_2$AlC. This is remarkably close to the prediction from the Fröhlich model. Using different Coulomb repulsion parameters ranging from 0.10 to 0.16 as before, the average $T_c$ is found be 5.651 K.
4. Summary

The structural properties of Nb$_2$AC ($A$: Al, S, Ge, As and Sn) compounds have been investigated and are summarized in tables 1 and 4. The calculated lattice parameters are in good accordance with previous experimental and theoretical studies, and the calculated electronic structure properties coincide very well with previous calculations. The electronic structure calculations reveal that the density of the states at the Fermi energy are mainly dominated by Nb 4d-states.

The phonon calculations show that the Nb$_2$AC ($A$: Al, S, Ge, As and Sn) materials are dynamically stable as no negative modes are observed. The high-frequency vibrations are dominated by C modes due to the light mass of C compared to the other elements, while the Nb, $A$ ($A$: Al, S, Ge, As and Sn) atoms dominate the low-frequency region due to their heavy mass. The phonon analysis is summarized in tables 2 and 5.

The calculated Eliashberg spectral function shows that the low-frequency phonon modes play a crucial role in the transition from the normal state to the superconducting state. These low-frequency modes are mainly due to the Nb and $A$ ($A$: Al, S, Ge, As and Sn) atoms, as expected from the electronic properties as all these atoms contribute significantly to $N(E_F)$. The calculated electron–phonon coupling parameter value are summarized in tables 3 and 6, and suggest a medium coupling strength for Nb$_2$AlC, Nb$_2$SC, Nb$_2$GeC and Nb$_2$SnC, and weak coupling strength for Nb$_2$AsC. By using the Allen–Dynes modified McMillan equation, the superconducting transition temperatures are found to be in good agreement with their experimental values (where available).

This work predicts that the previously unstudied Nb$_2$AlC is a superconductor with a transition temperature around 7 K. This work should also encourage the experimental and theoretical study of superconductivity in other Nb$_2$AC materials (e.g. $A$ = Ga, In, Tl, Pb etc) as in figure 6.

Acknowledgments

This work was supported by the Scientific and Technical Research Council of Turkey (TÜBİTAK) (2219 International Post Doctoral Research Fellowship Programme Project Number 1059B191900055). PJH was funded by an EPSRC RSE Fellowship (EPSRC Grant EP/R025770/1) PJB was funded by the UKCP High End Compute Consortium (EPSRC Grant EP/P022561/1). This project was undertaken on the Viking Cluster, which is a high performance compute facility provided by the University of York. We are grateful for computational support from the University of York High Performance Computing service, Viking and the Research Computing team.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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Table 6. DOS at the Fermi level ($N(E_F)$), logarithmic frequency ($\omega_{ln}$), the average electron–phonon coupling parameter ($\lambda$) and the superconducting transition temperature ($T_c$ in K) for the hexagonal Nb$_2$AlC for this work in bold, and their comparison with available previous experimental and theoretical results.

| Material    | $N(E_F)$ (states/eV) | $\omega_{ln}$ (K) | $\lambda$ | $T_c$ (K) |
|-------------|----------------------|-------------------|-----------|-----------|
| Nb$_2$AlC   | 3.316                | 322.951           | 0.646     | 6.709     |
| Exp [29]    |                      |                   | 0.460     |           |
| GGA [59]    | 3.400                |                   |           |           |
| GGA [64]    | 3.050                |                   |           |           |
| GGA [68]    | 3.360                |                   |           |           |
| LDA [58]    | 3.840                |                   |           |           |
| LDA [64]    | 2.920                |                   |           |           |
| LDA [67]    | 3.780                |                   |           |           |
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