Electronic structure, phonons, and electron-phonon interaction in Mo₃Si

H. M. Tütüncü,¹ S. Bağcı,¹ and G. P. Srivastava²

¹Fen-Edebiyat Fakültesi, Sakarya Üniversitesi, Fizik Bölümü, 54187 Adapazarı, Turkey ²School of Physics, University of Exeter, Stocker Road, Exeter EX4 4QL, United Kingdom (Received 17 September 2010: published 14 December 2010)

(Received 17 September 2010; published 14 December 2010)

The structural, elastic, electronic, dynamical, and superconducting properties of cubic A15 Mo_3Si have been investigated in detail by employing an *ab initio* pseudopotential method and a linear-response scheme within a generalized gradient approximation. In agreement with previous theoretical and experimental studies, it has been found that the Mo 4*d* states mainly contribute to the density of states very close to the Fermi level. The calculated phonon-dispersion relations for this material accord very well with the experimental data available along the principal symmetry directions. Our results show that the electron-phonon interaction in this material is much weaker than the corresponding interaction in other A15 materials, due the lower density of states at the Fermi level. The electron-phonon coupling parameter is found to be 0.453 and the superconducting critical temperature is estimated to be 1.27 K, in good agreement with the experimental value of 1.3 K.

DOI: 10.1103/PhysRevB.82.214510

PACS number(s): 74.25.Kc, 63.20.kd, 63.20.dk, 71.15.Mb

I. INTRODUCTION

The Mo-Si (molybdenum silicide) system has attracted a great deal of attention in the past 20 years since this system is of interest as high-reflectance x-ray optical elements,¹⁻³ gates, and interconnections in very large scale integrated circuits⁴⁻⁷ and high-temperature structural materials.⁸⁻¹⁴ Consequently, the structural, elastic, electronic, and vibrational properties of this system have studied by several groups. In particular, the phonon-dispersion curves and the phonon density of states of Mo₃Si have been measured by inelastic neutron spectroscopy.¹⁵ The electronic structure of this material has been investigated using a valence-band x-ray photoelectron spectroscopy.¹⁶ Nanoindentation techniques have been used to determine the elastic constants of Mo₃Si.¹⁷ In addition to this experimental work, measurements of the elastic constants for this material have also been reported in the Ph.D. thesis of Biragoni.¹⁸ On the theoretical side, full-potential muffin-tin orbital calculations (FP-LMTO) (Ref. 19) were reported for the bulk properties and density of states in Mo₃Si. This method was also used by Ma et al.²⁰ for obtaining electronic and elastic properties of Mo₃Si. The tight-binding study of thermal expansion for Mo₃Si was also presented in the work of Ma et al.²⁰ Recently, the heats of formation of stable and metastable phase of Mo-Si system were studied using the density-functional theory within a generalized gradient approximation (GGA).²¹

Although considerable progress has been made in experimental¹⁵ description of the vibrational properties of Mo_3Si , no *ab initio* results are available for the phonon spectrum and density of states. It is well known that a wide variety of physical properties of solids depend on their phonon properties, such as specific heats, thermal expansion, and heat conduction. Also, electron-phonon interaction plays an important role in determining the resistivity of metals and superconductivity. Thus, in view of the technological importance of this material, its static, elastic, electronic, and vibrational properties should be known clearly.

The aim of the present work is to investigate the structural, elastic, electronic, dynamical, and superconducting properties of cubic Mo₃Si by employing the plane-wave pseudopotential method, the density-functional theory, and a linear-response technique.^{22,23} The calculated structural parameters are compared with previous theoretical calculations and available experimental results. The peaks in the electronic density of states are compared with the corresponding peaks in the experimental work by Pankhurst *et al.*¹⁶ The phonon-dispersion relations and the superconducting critical temperature are favorably compared with the experimental results obtained by Christensen *et al.*¹⁵



FIG. 1. (a) The A15 structure of Mo_3Si . (b) Calculated total energies as a function of lattice constant in the cubic Mo_3Si .

Source	a (Å)	B (Mbar)	B'	C_{11} (Mbar)	<i>C</i> ₁₂ (Mbar)	C ₄₄ (Mbar)
This work	4.937	2.295	5.620	4.3852	1.251	1.064
Experimental (Ref. 11)	4.890					
LDA (Ref. 19)	4.840	2.534				
LDA+LMH (Ref. 19)	4.866	2.456				
FP-LMTO (Ref. 20)				5.390	1.470	1.180
Experimental (Ref. 17)				5.05 ± 0.35	0.80 ± 0.60	1.30 ± 0.15
Experimental (Ref. 18)		2.410		4.490	1.370	1.130

TABLE I. Structural parameters for Mo_3Si . The present results are compared with previous experimental and theoretical calculations.

II. DETAILS OF CALCULATIONS

The calculations are performed by employing the planewave pseudopotential method within the framework of the density-functional theory and a linear-response scheme,^{22,23} using the computing package QUANTUM ESPRESSO.²³ The electron-electron exchange-correlation interaction is described in the generalized gradient approximation using a functional proposed by Perdew and Wang, often referred to as PW91.^{24–26} To describe the electron-ion interaction, we have used ultrasoft pseudopotentials²⁷ for Mo and Si. The electronic wave functions were expanded in plane waves up to a maximal cutoff energy of 60 Ry. Self-consistent solutions of the Kohn-Sham equations were obtained by employing a set of Monkhorst-Pack special k points within the irreducible part of the Brillouin zone (IBZ). Since the crystal structure is metallic, convergence is reached using 176 special **k** points in the IBZ of the simple-cubic lattice.

A cubic crystal has three independent elastic constants: C_{11} , C_{12} , and C_{44} . The straightforward manner of obtaining these constants is to calculate the total-energy difference between an unstrained medium and a distorted medium at constant volume. We have used the volume-conserving tetragonal and monoclinic strains for $C_{11}-C_{12}$ and C_{44} , respectively.^{28,29} In order to obtain C_{11} and C_{12} separately, the relationship between these elastic constants and bulk modulus

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{1}$$

is also used. The calculations of the elastic constants require a very high degree of precision because the energy differences involved are on the order of less than 1 mRy. This circumstance requires the use of a fine **k**-points mesh. With our choice of a $(18 \times 18 \times 18)$ **k**-points grid the energy per atom was converged to 1 mRy or better in all cases. Moreover, the positions of atoms were relaxed during the volumeconserving tetragonal and monoclinic strain calculations.

Within the linear-response scheme, second-order derivatives of the total energy were calculated to obtain the dynamical matrix. A static linear response of the valance electrons was considered in terms of the variation in the external potential corresponding to periodic displacements of the atoms in the unit cell. The screening of the electronic system in response to the displacement of the atoms was taken into account in a self-consistent manner. Integration up to the Fermi surface is done with the smearing technique with the broadening parameter σ =0.015 Ry. For the Brillouin-zone integration we use the $8 \times 8 \times 8$ Monkhorst-Pack **k** mesh in the irreducible part of the Brillouin zone. We have calculated dynamical matrices at an uniform $4 \times 4 \times 4$ grid **q** points in the IBZ. Dynamical matrices at arbitrary wave vectors can be obtained by means of a Fourier deconvolution on this mesh.

We have also calculated the electron-phonon interaction parameter in Mo₃Si. The calculation of electron-phonon mass-enhancement parameter λ is explained clearly in several previous works.^{30–34} The value of λ leads us to calculate some parameters related to superconductivity. In general, $\langle \omega^n \rangle$ can be given as^{30–32,34}

$$\langle \omega^n \rangle = \frac{1}{\lambda} \sum_{\mathbf{q}j} \lambda_{\mathbf{q}j} \omega^n_{\mathbf{q}j}.$$
 (2)

The transition temperature T_C can be calculated from the Allen-Dynes modification of the McMillan formula^{30,31,34}

$$T_{C} = \frac{\omega_{\ln}}{1.2} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^{*}(1+0.62\lambda)}\right),$$
 (3)

where μ^* is the Coulomb pseudopotential, which describes the repulsive interaction between electrons. The values of



FIG. 2. The calculated electronic band structure for Mo_3Si . The Fermi level is set at 0 eV.



FIG. 3. The calculated total and partial electron density of states for Mo_3Si . The Fermi level is set at 0 eV.

this parameter vary between 0.12 and 0.16 in the literature.^{30–36} Thus, the effects of varying this parameter on the transition temperature T_C are studied in this work. The logarithmically averaged frequency ω_{ln} is expressed as

$$\omega_{\rm ln} = \frac{1}{\lambda} \sum_{\mathbf{q}j} \lambda_{\mathbf{q}j} \ln \omega_{\mathbf{q}j}. \tag{4}$$

Using T_C thus obtained, we calculate the gap energy (2 Δ) which is needed to break up a Cooper pair, from the relation

$$2\Delta = 3.53k_B T_C.$$
 (5)

III. RESULTS

A. Structural, elastic, and electronic properties

Mo₃Si has the A15 structure such as Cr₃Si, Cr₃O, Nb₃Al, Ti₃Sn, and Ti₃Au. Its crystal structure belongs to the space group $Pm\bar{3}n$ with Pearson symbol of cP8, and is shown in Fig. 1(a). There are eight atoms per unit cell, whose coordinates are

$$\begin{split} \tau_{\rm Si} &= (0.00, 0.00, 0.00), \\ \tau_{\rm Si} &= (0.50, 0.50, 0.50), \\ \tau_{\rm Mo} &= (0.25, 0.00, 0.50), \\ \tau_{\rm Mo} &= (0.75, 0.00, 0.50), \\ \tau_{\rm Mo} &= (0.50, 0.25, 0.00), \\ \tau_{\rm Mo} &= (0.50, 0.75, 0.00) \\ \tau_{\rm Mo} &= (0.00, 0.50, 0.25), \end{split}$$

and

$$\tau_{\rm Mo} = (0.00, 0.50, 0.75).$$

We have calculated the total energy at a number of lattice constants around the experimental value. The fitting of the calculated total-energy values to the Murnaghan equation of state is shown in Fig. 1(b). From this fit, we can obtain the equilibrium lattice constant (a), bulk modulus (B) and the pressure derivative of the bulk modulus (B'). The obtained equilibrium parameters (a, B, and B') are given in Table I, which also contains results of previous theoretical calculations as well as the experimental data. The elastic constants at the zero pressure are also listed in this table. All the calculated results accord with other theoretical calculations and available experimental data, implying the validity of the present work. In particular, compared with the experimental value¹¹ of 4.890 Å, we find a 0.96% overestimation for the lattice constant of the cubic Mo₃Si. The overestimation of the equilibrium lattice constant is a common feature with GGA calculations. Due to this overestimation, our calculations underestimate the bulk modulus of this material compared to its experimental value of 2.410 Mbar. The calculated elastic constants in Table I satisfy the mechanical stability conditions³⁷ in a cubic crystal, such as $C_{11} - C_{12}$ $>0, C_{11}>0, C_{44}>0, C_{11}+2C_{12}>0$, and $C_{12}<B<C_{11}$. Our results for the elastic constants are in good agreement with the experimental findings.^{17,18} The maximum difference between our calculations and experimental results has been found for C_{12} . Our calculated value for this elastic constant deviates from its experimental value¹⁸ of 1.370 Mbar within 9%. It is important to note that this difference is within typical experimental error margin.^{17,18}



FIG. 4. Phonon dispersion curves and density of states for Mo_3Si . Open circles present the presently calculated results while the filled squares show the experimental data from Ref. 15.

The calculated electronic structure along several highsymmetry directions of the simple-cubic Brillouin zone is displayed in Fig. 2. In this figure, the Fermi level is set to 0 eV. There are many bands crossing the Fermi level, suggesting that Mo₃Si shows metallic conductivity. Moreover, the energy bands around the Fermi energy are mainly derived from the 4d states of Mo atoms, indicating that these states dominate the conductivity of this material although d electrons are generally considered as less efficient conductors. In order to analyze the chemical bonding in the cubic Mo₃Si, we show the total and partial density of states for this material in Fig. 3. The peak at -8.9 eV is derived from Si 3s states with small contribution from the Mo 4d states. It is important to note that a similar observation has made in the theoretical as well as experimental work of Pankhurst et al.¹⁶ The peaks between -7 and 0 eV are dominated by hybridized Mo 4d and Si 3p states. Therefore, this material appears to have a covalent feature. The peaks above the Fermi level are mainly due to the Mo 4d states.

B. Phonons and electron-phonon interaction

In Fig. 4, the calculated phonon-dispersion curves are shown along several high-symmetry directions in the Brillouin zone. The total phonon density of states is shown on the right-hand side of this figure. The experimental phonon-dispersion data¹⁵ are indicated by filled squares. The presently calculated phonon spectrum agrees well with the experimental data,¹⁵ except for a small deviation for the highest optical phonon branch along the Γ -*X* direction. The computed transverse and longitudinal-acoustic (TA and LA) branches along the main symmetry directions of [100], [110], and [111] behave normally in the long-wave limit with steep slopes. This behavior leads us to calculate the elastics constants of Mo₃Si from the slopes of the acoustic branches in the phonon spectrum.³⁸ Along the [100] direction, the veloci-

ties of TA and LA branches are obtained to be 3337 m/s and 7226 m/s, respectively. These values leads us to calculate the elastic constants of C_{11} and C_{44} for Mo₃Si. Finally, C_{12} can be obtained by using these values and the velocity of LA phonon branch along the [110] direction (V_{LA} =6782 m/s). As a result, the values of C_{11} , C_{12} , and C_{44} are found to be 4.551, 1.525, and 0.971 Mbar. These values are comparable with our volume-conserving ab initio results as well as the experimental data^{17,18} in Table I. Figure 4 reveals that optical-phonon branches in Mo₃Si are distributed almost continuously from 4 to 10 THz. The optic branches between 4 and 8 THz are quite dispersive along the main symmetry directions [100], [110], and [111]. However, the optical branches above 9 THz show less dispersion and thus there is a large peak in the phonon density of states at 9.5 THz. We have observed an overlap of the acoustic and optical-phonon branches so that there is no visible gap in the phonon density of states. It can be seen from the critical assessment of this figure that there are three regions of importance in the density of states: (i) below 7.00 THz, (ii) 7.00-8.80 THz, and (iii) 8.80 THz onward. The peaks in the first and second regions are dominated by the vibrations of Mo and Si atoms. However, the peaks in the third region are mostly due to the vibrations of Si atoms with a small contribution from Mo vibrations. This is essentially due to the smaller mass of Si atoms. The zone-center phonon modes are of special importance in the lattice dynamics of solids since they can be detected by various experimental methods.

As mentioned before, the Mo₃Si cubic phase belongs to the $Pm\overline{3}n$ space group and the O_h³ point-group symmetries. Consequently, the zone-center atomic vibrations in this system can be decomposed as

$$\Gamma = T_{1u}^{1} + T_{1g} + T_{2u}^{1} + T_{2g} + A_{2g} + E_g + T_{1u}^{2} + T_{2u}^{2}$$

with the A, E, and T modes being singly, doubly, and triply degenerate, respectively. The vibrations of Mo atoms create



FIG. 5. Eigenvector representations of zone-center optical phonon modes in Mo₃Si.

the T_{1g} , T_{2g} , A_{2g} , and E_g phonon modes. For these phonon modes, Si atoms do not move. The lowest optical-phonon mode is due to the vibrations of atoms of both type with the maximum contribution coming from Mo atoms, as can be seen from Fig. 5. The T_{2u}^1 phonon mode also includes atomic vibrations from atoms of both type in the unit cell. Finally, the higher frequency modes T_{1u}^2 and T_{2u}^2 are mainly pictured by the vibrations of the lighter Si atoms.

The calculated Eliashberg spectral function is compared with the calculated phonon density of states in Fig. 6. This



FIG. 6. A comparison of the phonon density of states (dashed lines) and Eliashberg spectral function $\alpha^2 F(\omega)$ (solid lines).

figure indicates that the shape of the spectral function is quite similar to that of the density of states. From this spectral function, the electron-phonon mass-enhancement parameter λ is calculated to be 0.453. Taking typical values μ^* as 0.12, 0.13, 0.14, 0.15, and 0.16, T_C is determined to be 2.04 K, 1.63 K, 1.27 K, 0.97 K, and 0.72 K, respectively. All these values are within an acceptable range of the experimental value of 1.3 K.¹⁵ Using the value of λ , we have calculated other superconducting parameters, which are listed in Table II. Unfortunately, there are no experimental or theoretical results to compare our results. It is important to note that the T_C value for Mo₃Si is significantly lower than the corresponding values³⁶ for Nb₃Sn (T_C =18 K), Nb₃Al (T_C =18.6 K), Nb₃Ga (T_C =20.3 K), V₃Si (T_C =17.3 K), and V_3 Ga (T_C =23.0 K). All these materials crystallize in the A15 structure. We strongly believe that the reason for the smaller T_C for Mo₃Si can be linked to its lower density of states at the Fermi level $[N(E_F)=4.15 \text{ states/eV}]$, which, in turn, results in lower electron-phonon coupling parameter. In Table III, we have listed the electron-phonon coupling parameter (λ) as well as the density of states at the Fermi level $[N(E_F)]$ for different A15 materials.³⁶ This table clearly shows that the values of λ and T_C for Mo₃Si are much smaller than the corresponding values for other A15 materials due to its lower $N(E_F)$ value. It should be pointed out here that the results of T_C reported in Table III are subject to change for noncubic crystal phases of Mo₃Si. This is because the elastic stability condition $C_{11}-C_{12}>0$ is not guaranteed to hold for noncubic phases. In fact, the onset of the elastic instability upon a tetragonal distortion has recently been reported in V₃Si above T_C .³⁹

TABLE II. Superconducting parameters for Mo_3Si . Our T_C value is compared with its experimental value.

Source	μ	λ	$\langle \omega \rangle$ (K)	$\langle \omega^2 angle^{1/2}$ (K)	$\omega_{ m ln}$ (K)	<i>Т_С</i> (К)	2Δ (meV)
This work	0.14	0.453	127.87	191.67	379.92	1.27	0.388
Experimental (Ref. 15)						1.30	

Parameter	Mo ₃ Si	Nb ₃ Sn	Nb ₃ Al	Nb ₃ Ga	V ₃ Si	V ₃ Ga
$N(E_F)$ (states/eV)	4.15	11.66	14.65	14.10	14.72	19.61
λ	0.45	1.22	2.14	1.92	1.18	1.48
T_C (K)	1.27	12.6	14.8	22.5	18.4	23.0

TABLE III. The $N(E_F)$ (states/eV), λ and T_C (K) values for Mo₃Si. The values of these parameters for other A15 materials are taken from Ref. 36.

IV. SUMMARY

In this work, we have presented a detailed theoretical analysis of the structural, elastic and electronic properties for cubic Mo_3Si by using the generalized gradient approximation of the density-functional theory and *ab initio* pseudopotentials. Our results are in good agreement with experimental and previous theoretical results for lattice constant, bulk modulus, and second-order elastic constants. The electronic structure calculations clearly reveal the metallic nature of this material. The computed peaks and their origin in the electronic density of states are in good agreement with previous theoretical and experimental results.

The calculated phonon-dispersion relations for this material fit very well with the available experimental data. The polarizations of zone-center phonon modes are presented and discussed in detail. From the Eliashberg spectra function, the total electron-phonon coupling parameter (λ) is found to be 0.453. Using this value for λ , together with the choice $\mu^* = 0.14$ for the Coulomb pseudopotential, the transition temperature of this material is calculated to be 1.27 K, which compares very well with its experimental value of 1.3 K. A comparison of the calculated λ and T_C values for several A15 materials shows us that the electron-phonon interaction is comparatively much weaker in cubic Mo₃Si. This is due to its lower electronic density of states at the Fermi level.

ACKNOWLEDGMENT

The calculations reported here were performed using the University of Exeter's Intel Nehalem (i7) computer cluster.

- ¹A. K. Petford-Long, M. B. Stearns, C. H. Chang, S. R. Nutt, D. G. Stearns, N. M. Ceglio, and A. M. Hawrylak, J. Appl. Phys. **61**, 1422 (1987).
- ²D. G. Stearns, M. B. Stearns, Y. Cheng, J. H. Stith, and N. M. Ceglio, J. Appl. Phys. **67**, 2415 (1990).
- ³J. M. Slaughter, A. Shapiro, P. A. Kearney, and C. M. Falco, Phys. Rev. B **44**, 3854 (1991).
- ⁴K. Shibata, S. Shima, and M. Kashiwagi, J. Electrochem. Soc. 129, 1527 (1982).
- ⁵A. Perio and J. Torres, J. Appl. Phys. **59**, 2760 (1986).
- ⁶J. Y. Cheng, H. C. Cheng, and L. J. Chen, J. Appl. Phys. **61**, 2218 (1987).
- ⁷T. C. Chou and T. G. Nieh, Thin Solid Films **214**, 48 (1992).
- ⁸J. P. Meschter and D. S. Schwartz, J. Met. **41**, 52 (1989).
- ⁹A. K. Vasudévan and J. J. Petrovic, Mater. Sci. Eng., A **155**, 1 (1992).
- ¹⁰J. J. Petrovic, MRS Bull. 18, 35 (1993).
- ¹¹A. Misra, J. J. Petrovic, and T. Mitchell, Scr. Mater. **40**, 191 (1998).
- ¹²J. Chu, D. J. Thoma, K. J. McClellan, and P. Peralta, Mater. Sci. Eng., A **261**, 44 (1999).
- ¹³I. Rosales and J. H. Schneibel, Intermetallics **8**, 885 (2000).
- ¹⁴S. Ochiai, Intermetallics **14**, 1351 (2006).
- ¹⁵A. N. Christensen, J. E. Jorgensen, L. Pintschovius, F. Gompf, W. Reichardt, and N. Lehner, Phys. Rev. B 34, 2751 (1986).
- ¹⁶D. A. Pankhurst, Z. Yuan, D. Nguyen-Manh, M. L. Abel, G. Shao, J. F. Watts, D. G. Pettifor, and P. Tsakiropoulos, Phys. Rev. B **71**, 075114 (2005).
- ¹⁷J. G. Swadener, I. Rosales, and J. H. Schneibel, MRS Symposia Proceedings No. 646 (Materials Research Society, Pittsburgh,

2001).

- ¹⁸P. G. Biragoni, Ph.D. thesis, The Faculty of Mechanical Engineering Otto-von-University, 2007.
- ¹⁹A. K. McMahan, J. E. Klepeis, M. van Schilfgaarde, and M. Methfessel, Phys. Rev. B **50**, 10742 (1994).
- ²⁰N. Ma, B. R. Cooper, and B. S. Kang, J. Appl. Phys. **99**, 053514 (2006).
- ²¹Y. Chen, T. Hammerschmidt, D. G. Pettifor, J. Shang, and Y. Zhang, Acta Mater. **57**, 2657 (2009).
- ²²S. Baroni, P. Giannozzi, and A. Testa, Phys. Rev. Lett. 58, 1861 (1987).
- ²³S. Baroni, S. De Gironcoli, A. D. Corso, and P. Giannozzi, Rev. Mod. Phys. **73**, 515 (2001).
- ²⁴J. P. Perdew, in *Electronic Structure of Solids '91*, edited by P. Ziesche and H. Eschrig (Akademie, Berlin, 1991).
- ²⁵J. P. Perdew and Y. Wang, Phys. Rev. B **45**, 13244 (1992).
- ²⁶K. Burke, J. P. Perdew, and Y. Wang, in *Electronic Density Functional Theory: Recent Progress and New Directions*, edited by J. F. Dobson, G. Vignale, and M. P. Das (Plenum, New York, 1998).
- ²⁷D. Vanderbilt, Phys. Rev. B **41**, 7892 (1990).
- ²⁸M. J. Mehl, J. E. Osburn, D. A. Papaconstantopoulos, and B. M. Klein, Phys. Rev. B **41**, 10311 (1990).
- ²⁹P. Söderlind, O. Eriksson, J. M. Wills, and A. M. Boring, Phys. Rev. B 48, 5844 (1993).
- ³⁰W. L. McMillan, Phys. Rev. **167**, 331 (1968).
- ³¹P. B. Allen, Phys. Rev. B **6**, 2577 (1972).
- ³²W. Weber, Phys. Rev. B **8**, 5093 (1973).
- ³³R. Bauer, A. Schmid, P. Pavone, and D. Strauch, Phys. Rev. B

57, 11276 (1998).

- ³⁴S. Bağcı, H. M. Tütüncü, S. Duman, and G. P. Srivastava, Phys. Rev. B **81**, 144507 (2010).
- ³⁵R. C. Dynes and C. M. Varma, J. Phys. F: Met. Phys. **6**, L215 (1976).
- ³⁶B. M. Klein, L. L. Boyer, and D. A. Papaconstantopoulos, Phys.

Rev. Lett. 42, 530 (1979).

- ³⁷M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Clarendon, Oxford, 1956).
- ³⁸G. P. Srivastava, *The Physics of Phonons* (Adam Hilger, Bristol, 1990).
- ³⁹C. Paduani and C. A. Kuhnen, Eur. J. Phys. B 66, 353 (2008).