3. Theoretical models

Comparison of theoretical results with experiment is hampered by the fact that the earlier measurements did not include enough information. The later measurements [73Ro1, 76St1] showed the importance of three body interactions. Beryllium is a simple metal where standard pseudopotential perturbation theory should be applicable. The usual second order calculations however, yield only pair forces. A third order calculation was done by Bertoni et al. [75Be3]. The general shape of the curves is in good agreement with the experimental data. There is a large difference between the second and third order results by these authors which seems to indicate a slow convergence of the perturbation series, see Fig. 3 Be. No adequate fit of the latest experimental data has been published so far.

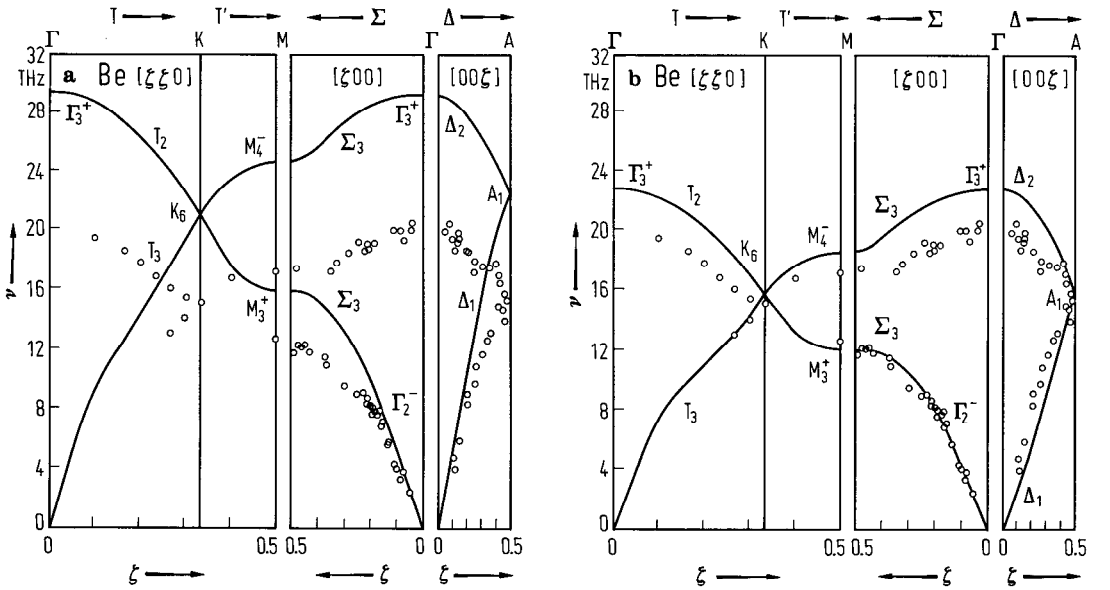


Fig. 3 a, b. Be. Theoretical phonon frequencies in high symmetry directions for modes polarized perpendicularly to the basal plane. a) second order pseudopotential perturbation theory b) third order theory. The experimental points are taken from [66Sc1] and [73Ro1], [75Be3].

Born-von Karman and equivalent models: [65De1, 66Sc3, 71Sr1], further references: [69Me1, 71Be1, 71Tr2, 78Ku5].

Short ranged forces plus a simple electronic contribution: [73Ku1], further references: [62Sc1, 70Sh2, 71Ku1, 73Bo1, 73Ra2, 73Up1, 78Mi1].

Pseudopotential calculations: [75Be3, 69Br1, 75Ha2], further references: [66Sa1, 69Gi1, 69Ki1, 69Sa1, 70Ki1, 70Pr2, 75Ma1, 76Da1].

Bi Bismuth

Lattice: rhombohedral (A7), $a = 654$ pm $= 6.54$ Å, $\alpha = 87°34'$. BZ: see p. 453.

1. Phonon dispersion

Table 1. Bi. Measurements.

Method	T [K]	Fig.	Ref.
neutron diffraction (TAS)	75	1 Bi	Macfarlane [71Ma1]
neutron diffraction (TAS)	75		Smith [67Sm1]
neutron diffraction (TAS)	296		Sosnowski et al. [68So1]

Further measurements: [64Ya1].

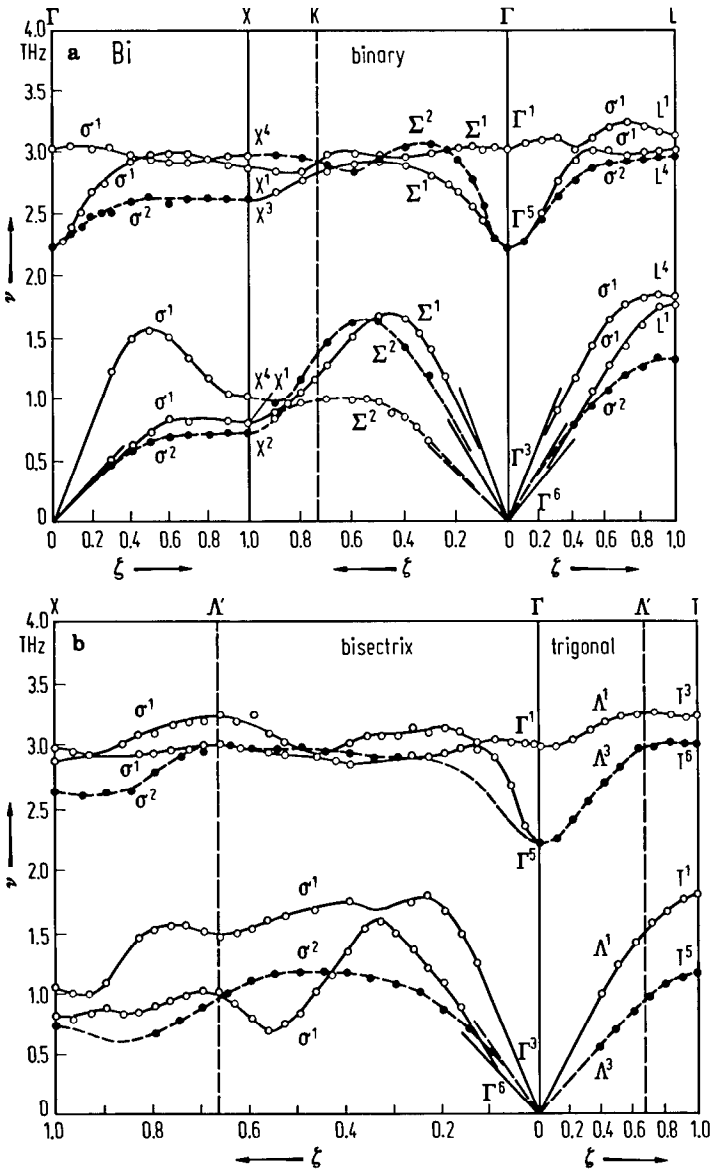


Fig. 1a, b. Bi. Measured phonon dispersion curves at 75 K. The initial slopes of the acoustic modes were computed from the elastic constants [60Ec1]. The smooth curves shown are only guides to the eye [71Ma1].

The dispersion curves of bismuth resemble those of As and Sb. The group theory for these elements was reported in [67Sm1]. The optical frequencies at the Γ point are in good agreement with the values obtained from Raman scattering [73Ro1, 75La2]. The decrease of these frequencies with increasing temperatures is small $\nu(T=80\,\mathrm{K}) = \nu(T=300\,\mathrm{K}) = 0.05$ THz for (Γ^5) and 0.09 THz for (Γ^1), respectively. A five neighbour Born-von Karman model gives a good overall description of the dispersion, whereas it is estimated that an accurate fit would need forces to the 25th neighbours (at least 50 parameters).

Table 2. Bi. Measured phonon frequencies. The estimated random error in any particular frequency is 2···4 %.

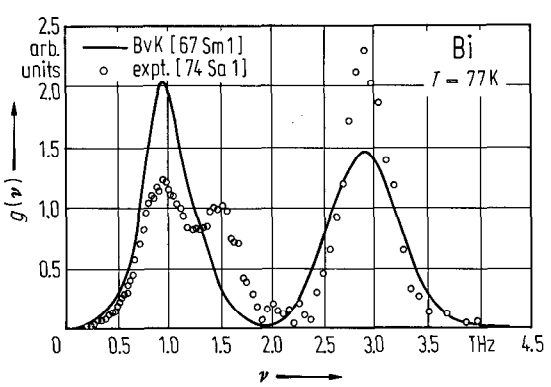
Ref.	64Ya1							
T	75 K	300 K	75 K	300 K	75 K	300 K	75 K	300 K
ζ	ν [THz]							
	$\Gamma \rightarrow T$ (trigonal)							
	Λ_3(TA)	Λ_3(TA)	Λ_3(TO)	Λ_3(TO)	Λ_1(LA)	Λ_1(LA)	Λ_1(LO)	Λ_1(LO)
0.0			2.33	2.16			3.02	2.99
0.1			2.26	2.24			3.01	3.01
0.2			2.40	2.40			3.06	2.98
0.3			2.56	2.56			3.14	3.07
0.4	0.56	0.57	2.72	2.72	0.99	0.99	3.20	3.14
0.5	0.69	0.70	2.85	2.83	1.22	1.23	3.25	3.18
0.6	0.83	0.83	2.99	2.93	1.41	1.40	3.26	3.26
0.7	0.96	0.95	2.99	2.96	1.57	1.54	3.28	3.21
0.8	1.06	1.05	3.04	2.98	1.66	1.66	3.26	3.20
0.9	1.12	1.10	3.06	3.04	1.77	1.75	3.23	3.17
1.0	1.16	1.11	3.04	3.01	1.80	1.80	3.25	3.21

Ref.	67Sm1					
T	75 K					
ζ	ν [THz]					
	$\Gamma \rightarrow K \rightarrow X$ (binary)					
branch	Σ_1(A)	Σ_1(O)	Σ_1(O)	Σ_2(A)	Σ_2(A)	Σ_2(O)
0.0		2.23	3.02			2.23
0.1						
0.2	1.10					
0.3	1.50			0.53	0.72	
0.4	1.67	2.85		0.64	0.84	
0.5	1.64	2.94			0.95	
0.6	1.48	2.99		0.89	0.94	2.86
0.7	1.27	2.93				
0.8	1.15	2.97			1.02	2.86
0.9		2.67		0.89		
1.0	0.95	2.66	3.02	0.80	1.03	2.86

(continued on next page)

2. Frequency spectra and related properties

Frequency spectra of bismuth at 77 K and 296 K: see Figs. 2 Bi and 3 Bi.



◀ Fig. 2. Bi. Phonon frequency spectrum at 77 K measured by coherent inelastic neutron scattering of a polycrystalline sample. The spectrum calculated from a Born-von Karman model of [67Sm1] folded with the experimental resolution [74Sa1] is also shown.

Table 2. Bi (continued)

Ref.	67Sm1					
T	75 K					
ζ	ν [THz]					
	$\Gamma \rightarrow X$					
branch	σ_1(A)	σ_1(A)	σ_1(O)	σ_1(O)	σ_2(TA)	σ_2(TO)
0			2.23	3.02		2.33
0.1			2.39			
0.2			2.67	2.99		2.51
0.3		1.21				
0.4	0.59	1.45	2.91	2.98	0.64	2.63
0.5	0.73	1.53	2.94			
0.6	0.83	1.46	2.90	2.94	0.75	2.67
0.7		1.34				
0.8	0.94	1.16	2.85	3.02	0.78	2.69
0.9		1.05		2.94		
1.0	0.95	1.03	2.86	3.02	0.80	2.66

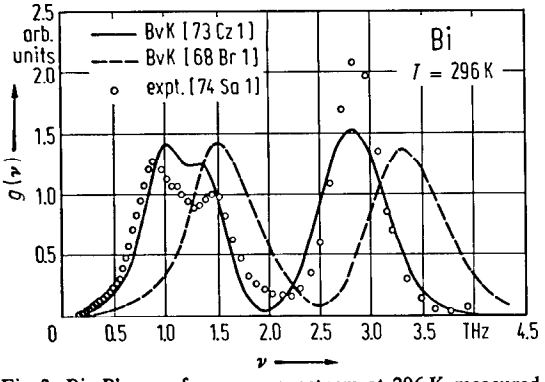


Fig. 3. Bi. Phonon frequency spectrum at 296 K measured by coherent inelastic neutron scattering of a polycrystalline sample. Two spectra calculated from Born-von Karman models folded with the experimental resolution [74Sa1] are also to be seen.

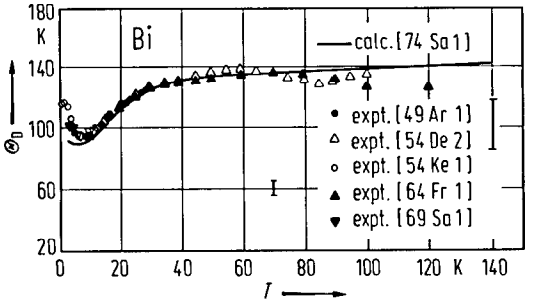


Fig. 4. Bi. Debye temperatures Θ_D calculated from the experimental spectrum of Fig. 2 Bi compared to experimental values [74Sa1].

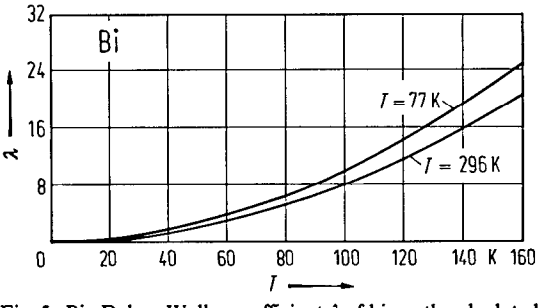


Fig. 5. Bi. Debye-Waller coefficient λ of bismuth calculated from the experimental spectra of Figs. 2 Bi and 3 Bi [74Sa1].

3. Theoretical models

The models reproduce only roughly the overall shape of the dispersion curves.
Born-von Karman models: [67Sm1, 73Cz1, 68Br1].

Sb Antimony

Lattice: rhombohedral (A7), $a = 622$ pm $= 6.22$ Å, $\alpha = 87° 24'$. BZ: see p. 453.

1. Phonon dispersion

Table 1. Sb. Measurements.

Method	T [K]	Fig.	Ref.
neutron diffraction (TAS)	295	1 Sb	Sharp and Warming [71Sh4]
neutron diffraction (TAS)	≈300		Sosnowski et al. [72So1]

Further measurements: [71So1, 63Fo1].

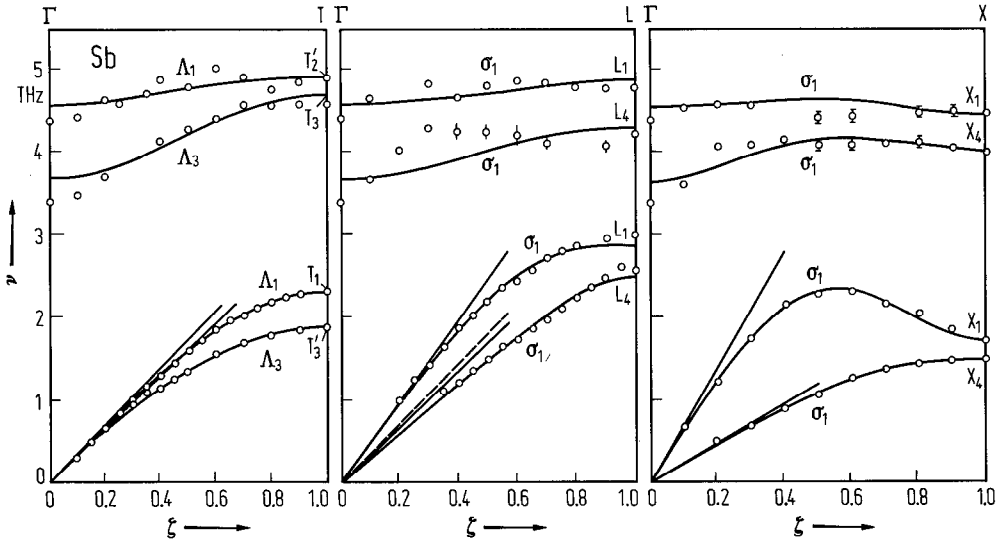


Fig. 1. Sb. Measured phonon dispersion at 295 K. The smooth curves are given by the result of a ninth neighbour Born-von Karman model [71Sh4].

The dispersion curves of antimony are similar to the ones of Bi. The group theory for these elements was reported in [67Sm1]. The optical frequencies at the Γ point are in good agreement with the values measured by Raman scattering [75La2]. A ninth nearest neighbour Born-von Karman model gives a good overall description of the measured dispersion and a reasonable agreement with the measured spectrum.

2. Phonon spectrum and related properties

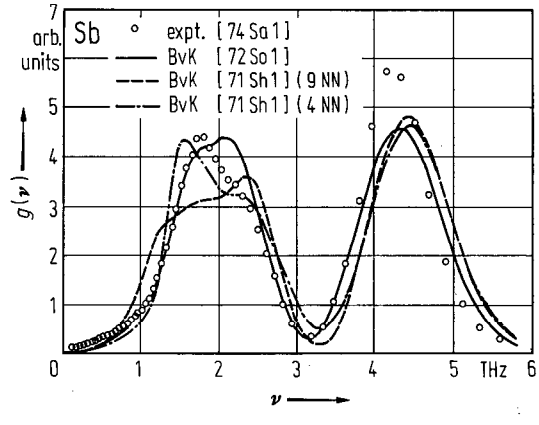


Fig. 2. Sb. Phonon spectrum measured by inelastic coherent scattering on a polycrystalline sample compared to spectra obtained from Born-von Karman fits to the measured dispersion curves and folded with the experimental resolution [74Sa1]. (error: 71Sh1 should read 71Sh4).

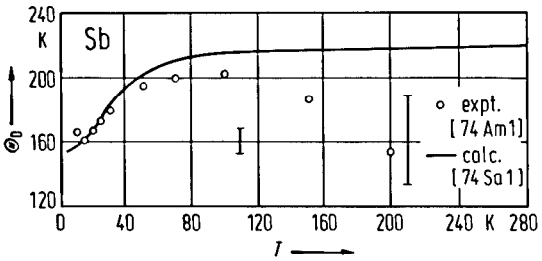


Fig. 3. Sb. Debye temperature Θ_D calculated from the experimental spectrum of Fig. 2 Sb compared to experimental values [74Sa1].

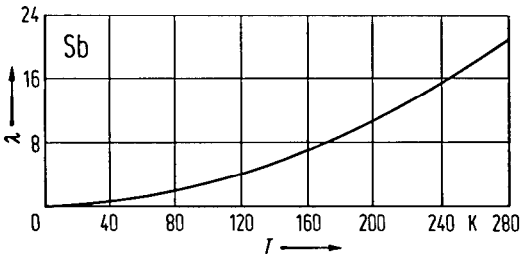


Fig. 4. Sb. Debye-Waller coefficient λ calculated from the experimental spectrum of Fig. 2 Sb [74Sa1].

3. Theoretical models

Born-von Karman models [71Sh4, 72So1].

Sc Scandium

Lattice: hcp, $a = 331$ pm $= 3.31$ Å, $c = 527$ pm $= 5.27$ Å. BZ: see p. 450.

1. Phonon dispersion

Table 1. Sc. Measurements

Method	T [K]	Fig.	Ref.
neutron diffraction (TAS)	295	1 Sc	Wakabayashi et al. [71Wa1]

The phonon dispersion curves of scandium are similar to the ones of yttrium. They yield long range interactions in the basal plane but interactions which decrease rapidly in the direction normal to the basal plane. One Kohn type anomaly was found.

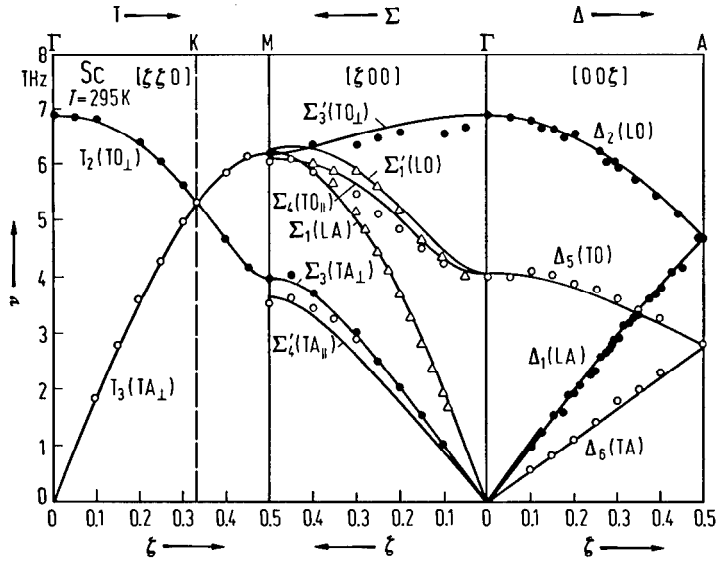


Fig. 1. Sc. Measured phonon dispersion curves at 295 K. The lines correspond to the sixth neighbour Born-von Karman model of Table 3 Sc [70Wa1].