

## Phonon dispersion of $\beta$ -Sc

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The phonon dispersion has been measured in the high-temperature bcc phase of a group-III metal (one  $d$  electron). In spite of its simple monatomic Bravais lattice the vibrational behavior of  $\beta$ -Sc is very anisotropic: a valley of low-energy and strongly damped phonons extends along the Brillouin-zone surface. These large-amplitude vibrations displace the lattice towards the stacking sequence of the low-temperature hcp phase and the hitherto unobserved  $\omega$  structure, and are interpreted as *dynamical* precursor fluctuations towards the reconstructive phase transitions.

### INTRODUCTION

A considerable fraction of the metallic elements on the left side of the Periodic Table solidifies in the open bcc structure. With a few exceptions, these bcc structures transform either by lowering the temperature or under pressure to close-packed structures. Most of these transitions are supposed to be displacive first-order transitions.

The sequence of transition elements from groups III to VI may serve as an illustration. The group-III metals, Sc, Y, and La form a hcp ( $\alpha$ ) lattice at low temperature and transform to a bcc ( $\beta$ ) lattice only in a narrow temperature range below melting.<sup>1</sup> For instance, Y crystallizes to a bcc lattice only during the last 40 K below its melting point. With increasing  $d$ -electron density, the range of existence of the bcc phase increases: In the group-IV metals Ti, Zr, and Hf, the bcc structure exists over the upper third of the temperature range of the solid phase, and in group-V and -VI metals, the bcc structure is the stable structure over the whole temperature range of the solid state. As a parallel, the melting temperature increases to exhibit in W the highest melting point of a pure metal. Whereas the stability of the ground state, i.e., the sequence of hcp to bcc, is well understood in models using the  $d$ -electron density as a control parameter,<sup>2</sup> the reason for stabilizing the bcc structure at high temperature, where ground-state calculations predict close-packed structures, is less evident. In general, it is agreed that an increase of vibrational entropy<sup>3</sup> at the transition stabilizes the bcc structure. Alternatively, an increase of the electronic entropy has been proposed.<sup>4</sup>

Knowledge of the vibrational behavior of these bcc structures is then the key information needed to understand its varying stability. Furthermore, we expect to learn about the transformation path to a close-packed structure. A series of phonon-dispersion measurements

of the bcc phase of the group-IV metals<sup>5-7</sup> gave an answer. A valley of low-energy and strongly damped vibrations causes a large vibrational entropy and is the dominant contribution in stabilizing the bcc structure in group-IV metals. Furthermore, the eigenvectors of these large-amplitude vibrations are all involved in the displacive phase transition.<sup>8</sup>

### EXPERIMENTAL CONSIDERATIONS

Here we present a complete phonon-dispersion measurement in the bcc phase of a group-III metal, i.e.,  $\beta$ -Sc with a range of existence from  $T_{\alpha\beta}=1610$  K to  $T_m=1814$  K. It is this reconstructive or martensitic phase transition which has so far prevented access to the large bcc single crystals needed to measure the phonon dispersions. We have overcome this problem by the *in situ* growth of single crystals<sup>9</sup> on a three-axis spectrometer and subsequently performed phonon measurements without cooling the crystal below the transition temperature. The latter unavoidably destroys the single crystal into different grains according to the different variants of the Burgers transformation scheme. From high-purity (4N) Sc rods of 8 mm in diameter, several 3–5-cm-long single crystals could be grown by a crucible free-zone melting technique<sup>6,9</sup> and oriented without cooling below the transition temperature. To avoid the evaporation of the sample—Sc has a vapor pressure of  $\sim 0.12$  mbar at  $T_m$ —an inert gas atmosphere of 900 mbar of 6N Ar has been used. The inelastic neutron measurements have been performed by means of the three-axis spectrometers IN8 and IN3 of the Institut Laue-Langevin using predominantly graphite monochromators and analyzers, a horizontal collimation of 40', 40', 40', 40', and a graphite filter to suppress  $\lambda/2$  contaminations. Density-of-states peaks, due to the considerable incoherent cross section

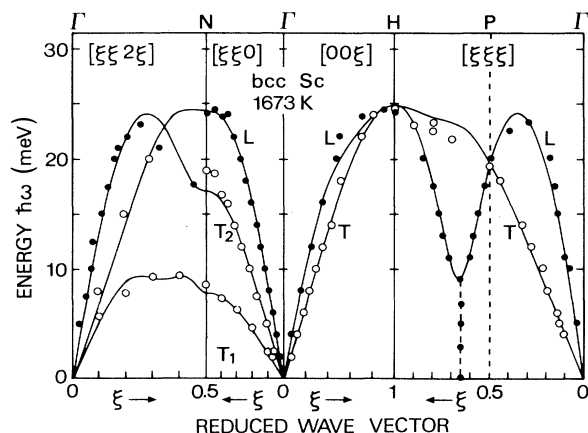


FIG. 1. Phonon dispersion of  $\beta$ -Sc at 1673 K. The solid lines represent a Born-von Kármán fit with force constants up to the fifth nearest-neighbor shell.

$\sigma_{\text{inc}} = 4.5(5)$  b of Sc, made it difficult but not impossible to evaluate some of the phonon peaks near the Brillouin-zone boundary. A lattice parameter  $a = 3.765(5)$  Å at 1673 K has been measured.

## RESULTS AND DISCUSSION

Figure 1 and Tables I and II show the so-determined phonon dispersion of  $\beta$ -Sc at 1673 K. The most striking result is its resemblance to those of the group-IV metals  $\beta$ -Ti,  $\beta$ -Zr, and  $\beta$ -Hf. (i) The longitudinal  $L[\xi\xi\xi\xi]$  phonon branch shows a pronounced dip at  $\xi = \frac{2}{3}$ . The intensity of inelastic origin is measured here down to zero-energy transfer. (ii) The transverse  $T_1[\xi\xi 0]$  branch with  $[1\bar{1}0]$  polarization is of low frequency. (iii) The  $L\frac{2}{3}(111)$

and the  $T_1\frac{1}{2}(110)$  phonon at the  $N$  point are connected via a valley of low-energy and transverse zone-boundary phonons along  $[\xi\xi 2\xi]$ .<sup>5</sup> (iv) All these low-energy phonons, i.e., the  $L\frac{2}{3}(111)$ , the  $T_1[\xi\xi 0]$ , and the  $T_1[\xi\xi 2\xi]$  phonon branches, are strongly damped. Figure 2 gives an impression of this damping.<sup>10</sup> Already, at small  $\xi \approx 0.1$ , phonon groups start to broaden and show a maximum broadening in between  $T_1\frac{1}{3}(112) \equiv L\frac{2}{3}(111)$  and the  $N$  point [ $T_1\frac{1}{2}(112) \equiv T_1\frac{1}{2}(110)$ ].

As argued in our previous work,<sup>5</sup> these broad excitation distributions can be adequately described by a damped oscillator with a damping term  $\Gamma$ , which accounts, via the uncertainty relation, for the finite phonon lifetime. In particular, the damped oscillator describes the intensity of inelastic origin reaching down to zero-energy transfer. This has to be separated from the purely elastic-scattering events originating from either spin incoherent scattering or diffuse elastic scattering of coherent origin. Figure 2 shows that the broad intensity distributions are remarkably well reproduced by the line shape of the damped oscillator, including a purely elastic peak on top of the distribution (see Table II). Because of the smooth variation of the intensity of this peak with the scattering vector  $Q$  (caused by the Debye-Waller factor), it can be clearly ascribed to incoherent scattering. Its width is a measure of the energy resolution of the spectrometer. The absence of any diffuse elastic intensity of coherent origin leads then to the conclusion that the strongly damped and large-amplitude fluctuations do not condense to static displacements within the time window of the method ( $\sim 0.5 \times 10^{-11}$  s). Narrowing the time window, e.g., using the poor energy resolution of x-ray scattering, these fluctuations would reappear as elastic diffuse scattering. Now its absence shows that no static embryos of the new phase exist within the mother phase. This confirms the picture that in the absence of point defects, precursors of the reconstructive or martensitic phase transitions, at least in the group-III and -IV metals,

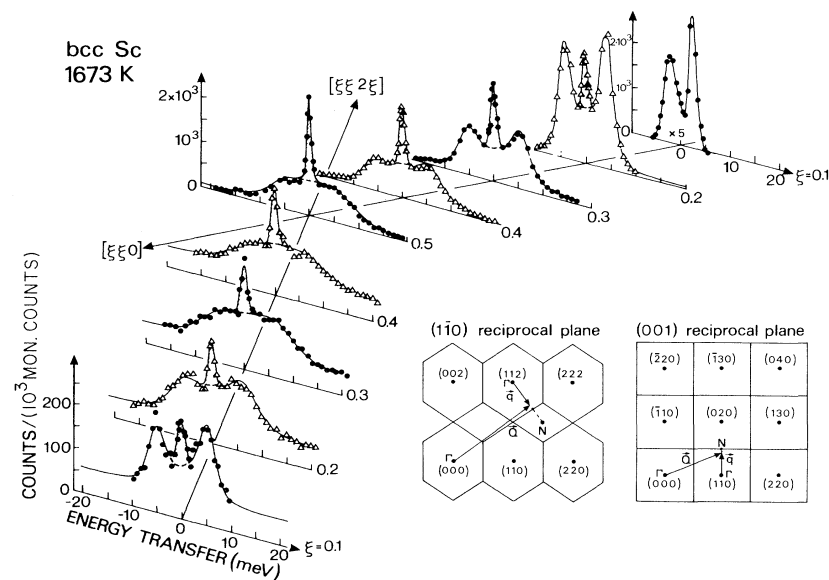


FIG. 2. Phonon spectra of the  $T_1[\xi\xi 0]$  and  $T_1[\xi\xi 2\xi]$  phonon branch in  $\beta$ -Sc at 1673 K. The solid lines show fits with a damped oscillator function. The peak on top of the broad phonon groups originates from elastic incoherent scattering.

are of purely dynamical nature.<sup>8</sup>

Whereas from  $Q = \frac{4}{3}(111)$  broadened phonons extend along  $[\xi\xi 2\xi]$  in reciprocal space, they are confined to a narrow band in the  $[\xi\xi\xi]$  direction. This becomes evi-

dent from Fig. 3 where constant-energy scans centered around  $Q = \frac{4}{3}(111)$  and along  $[\xi\xi\xi]$  are shown.

$\beta$ -Sc shows all the dynamical precursors of the  $\beta$ -to- $\alpha$  transition, which we know from the group-IV metals.

TABLE I. Phonons in  $\beta$ -Sc; errors refer to statistical errors only.

$\xi$		$\hbar\omega$ (meV)	$\xi$	$\hbar\omega$ (meV)
	$L[\xi\xi\xi]$			
0.037(1)		5.0	0.346(8)	12.0
0.038(1)		5.0	0.43(1)	14.0
0.077(4)		10.0	0.509(8)	18.0
0.142(5)		15.0	0.696(8)	22.0
0.155(7)		17.5	0.70	22.5(5)
0.19(2)		20.0	0.8	24(1)
0.3		23.2(4)		
0.4		22.5(4)		
			$L[\xi\xi 0]$	
0.492(5)		20.0	0.018(2)	2.0
0.530(5)		17.5	0.046(1)	4.0
0.565(5)		15.0	0.070(1)	6.0
0.592(5)		13.0	0.095(1)	8.0
0.605(3)		11.0	0.124(1)	10.0
0.657(3)		9.0	0.150(2)	12.0
0.655(2)		7.0	0.179(3)	14.0
0.651(2)		5.0	0.210(3)	16.0
0.651(2)		3.0	0.250(3)	18.0
0.654(2)		0.0	0.282(4)	20.0
0.717(3)		11.0	0.327(6)	22.0
0.750(5)		13.0	0.369(6)	24.0
0.772(3)		15.0	0.4	23.8(2)
0.77(1)		16.0	0.45	24.5(3)
0.797(5)		17.5	0.5	24.1(3)
0.853(7)		20.0	0.5	24.5(1.0)
1.0		24.1(5)		
			$T_2[\xi\xi 0]$	
	$T[\xi\xi\xi]$		0.059(1)	2.5
0.105(5)		4.0	0.110(1)	5.0
0.13(1)		5.0	0.173(2)	7.5
0.142(5)		6.0	0.220(4)	10.0
0.196(5)		8.0	0.275(6)	12.0
0.219(9)		10.0	0.321	14.0
0.283(6)		12.0	0.36(1)	16.0
0.329(5)		14.0	0.4	16.8(4)
0.45(1)		18.0	0.45	18.7(4)
0.8		22.5(1.2)	0.5	19.1(1)
			0.5	17.5(3)
	$L[00\xi]$		0.5	20.4(2)
0.066(1)		4.0	0.5	19.8(5)
0.153(2)		8.0		
0.248(5)		12.0	0.027(3)	5.0
0.346(7)		16.0	0.026(1)	5.0
0.463(15)		20.0	0.044(3)	7.5
0.50(2)		22.0	0.050(5)	7.5
0.7		23.8(6)	0.069(3)	10.0
0.9		24.4(1.0)	0.074(5)	12.5
			0.105(12)	15
	$T[00\xi]$		0.132(7)	17.5
0.071(1)		2.0	0.153(5)	20.0
0.100(5)		4.0	0.165(4)	21
0.112(3)		4.0	0.20(1)	22
0.187(5)		6.0	0.25	23(2.5)
0.174(5)		6.0	0.321(17)	21
0.226(5)		8.0	0.45	18(4)
0.289(7)		10.0		
			$L[\xi\xi 2\xi]$	

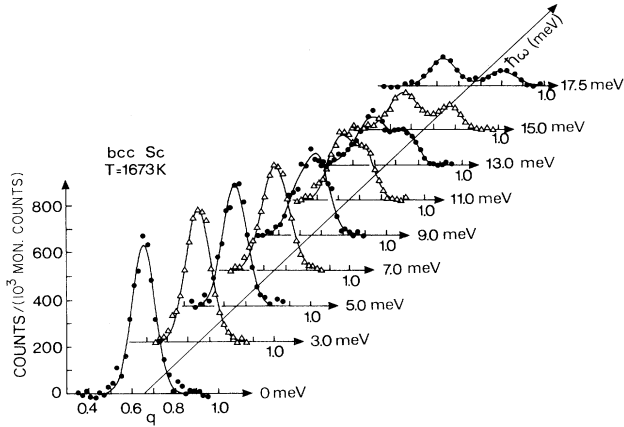


FIG. 3.  $Q$  scans for  $\beta$ -Sc around  $Q = \frac{4}{3}(111)$  and with  $q \parallel [\xi\xi\xi]$ . The elastic and inelastic incoherent scatterings have been subtracted. The remaining intensity at zero-energy transfer is due to the strong damping of the  $L_{\frac{2}{3}}^2(111)$  phonon. Fits with one or two Gaussians of nearly constant full width at half maximum (FWHM)  $\approx 0.1$  r.l.u. are shown. The dots in Fig. 1 along the hatched line at  $L_{\frac{2}{3}}^2(111)$  correspond to the peak positions.

The  $T_{1\frac{1}{2}}(110)$  phonon, which shuffles the (110) bcc planes into the stacking sequence of the hcp basal planes in the  $\alpha$  phase, is of very low energy and therefore of large amplitude. The initial slope of the  $T_1[\xi\xi 2\xi]$  phonon branch is low and thereby indicates a low resistivity for (112)  $[11\bar{1}]$  shears. A combination of two of these shears squeezes the bcc octahedron to the regular octahedron of hcp structure.

Whereas dynamical precursors toward the  $\alpha$  phase were expected in  $\beta$ -Sc, the strong dip at  $L_{\frac{2}{3}}^2(111)$  (the intensity of inelastic origin reaches down to zero-energy transfer; see Fig. 3) was to a certain extent unexpected. This mode displaces out of three neighboring (111) planes two planes toward each other, whereas the third stays at rest. Assuming that the two oscillating planes collapse, the hexagonal (but not close packed)  $\omega$  structure is formed. This structure is known under pressure for the group-IV metals.<sup>11</sup> The longitudinal  $L_{\frac{2}{3}}^2(111)$  mode is equivalent to the transverse  $T_{1\frac{1}{3}}(112)$  mode and can therefore be viewed as a shearing motion of neighboring  $[111]$  chains. The systematics within the transition metals predict for elements with only one  $d$  electron low restoring forces for a shearing of  $[111]$  chains against each other.<sup>8</sup> However, to our knowledge, no formation of the  $\omega$  structure under pressure or alloying has been reported so far. The close resemblance to the  $\omega$  phonons in the group-IV metals suggests that  $\beta$ -Sc shows a similar tendency to transform to the  $\omega$  structure. We therefore expect the existence of the  $\omega$  phase in Sc—and presumably in the other group-III elements as well—either under pressure or from alloying.

The phonon dispersion has been parametrized by a

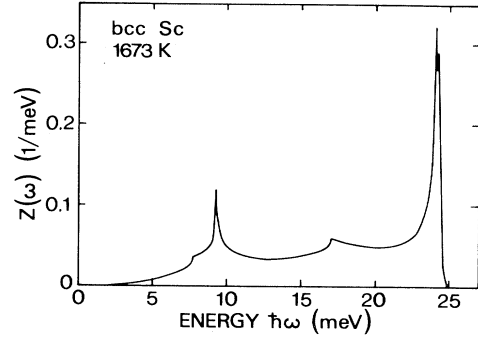


FIG. 4. Phonon density of states,  $Z(\omega)$ , for  $\beta$ -Sc at 1673 K.

Born–von Kármán (BvK) fit with force constants  $\phi_{ij}^m$  up to the fifth nearest-neighbor shell (Table III), which again have been used to calculate the phonon density of states,  $Z(\omega)$ , within a (quasi)harmonic approximation as shown in Fig. 4.  $Z(\omega)$  of  $\beta$ -Sc shows the same structure as those of the group-IV metals.

$Z(\omega)$  allows then the computation of the lattice entropy  $S_{\text{vib}}$ :

$$S_{\text{vib}} = -3k_B \int_0^\infty d\omega Z(\omega) [n(\omega) \ln n(\omega) - \{1 + n(\omega)\} \ln \{1 + n(\omega)\}], \quad (1)$$

where  $n(\omega) = (e^{\hbar\omega/k_B T} - 1)^{-1}$ . Compared to the group-V and -VI metals, which have a bcc structure all over the temperature range of the solid state,  $\beta$ -Sc has a particular high lattice entropy  $S_{\text{vib}} = 9.6k_B/\text{atom}$  at 1673 K (see Table IV). This high value is caused by the low-energy phonons at the Brillouin-zone boundary and is a strong hint that the bcc phase is stabilized mainly by the increase of  $S_{\text{vib}}$  at the phase transition. A comparison of phonons from the  $\beta$  phase with those of the  $\alpha$  phase<sup>12,13</sup> supports this idea. For instance, in  $\alpha$ -Sc the energy of the transverse-optical mode at the  $\Gamma$  point is twice the energy of the corresponding bcc phonon. This mode in the  $\alpha$  phase performs a shearing of successive hcp basal planes in opposite directions which corresponds in the

TABLE II. Phonons in  $\beta$ -Sc at 1673 K fitted with a damped oscillator function.

$\xi$	$T_1[\xi\xi 0]$		$T_1[\xi\xi 2\xi]$	
	$\hbar\omega_0$ (meV)	$\Gamma$ (meV)	$\hbar\omega_0$ (meV)	$\Gamma$ (meV)
0.1	2.47(1)	0.62(2)	5.7(2)	3.4(5)
0.2	4.62(5)	2.5(1)	7.8(2)	7.8(5)
0.3	6.29(8)	5.0(2)	9.3(5)	11.8(1.3)
0.4	7.30(15)	7.7(4)	9.4(6)	12.8(1.7)
0.5	8.5(1.4)	11.8(—)		

TABLE III. Interatomic force constants  $\phi_{ij}^m$  in bcc Sc in units of N/m, obtained from a Born–von Kármán fit to the dispersion including the five nearest-neighbor shells.

$1_{xx}$ : 6.377	$1_{xy}$ : 6.613	$2_{xx}$ : 2.890	$2_{yy}$ : -0.347	$3_{xx}$ : -0.002
$3_{zz}$ : -0.849	$3_{xy}$ : -0.035	$4_{xx}$ : 0.406	$4_{yy}$ : -0.081	$4_{yx}$ : -0.704
$4_{xy}$ : 0.086	$5_{xx}$ : 0.263	$5_{xy}$ : 0.456		

bcc structure to the  $T_{1\frac{1}{2}}(110)$  shearing. The argument that the excess entropy at the phase transition is mainly of vibrational origin is speculative because the lattice entropy of the  $\alpha$  phase at  $T_{\alpha\beta}$ , which has to be compared to the corresponding entropy of the  $\beta$  phase, is not reliably known. Presumably, the phonon frequencies in  $\alpha$ -Sc decrease when approaching the phase transition from low temperatures, as known from the group-IV metals.<sup>14</sup> Therefore the lattice entropy of  $\alpha$ -Sc will increase beyond the harmonic estimation [Eq. (1)] based on the only available room-temperature phonon dispersion.<sup>12,13</sup> Phonon measurements in  $\alpha$ -Sc close to  $T_{\alpha\beta}$  would solve the problem.

The particular importance of the low-energy excitations in  $\beta$ -Sc is also reflected in a considerable decrease of the Debye temperature  $\Theta_D$  (Table IV) as calculated from  $Z(\omega)$  when compared to that of  $\alpha$ -Sc.

The elastic constants at 1673 K have been calculated from the force constants  $\phi_{ij}^m$ .<sup>15</sup> Similar to the group-IV metals and despite the high symmetry of the bcc structure,  $\beta$ -Sc shows a pronounced anisotropy factor  $C_{44}/C' = 4.1$  for the two independent shear moduli (see Table IV).

The parametrization of the measured phonon dispersion by a BvK fit does not take into account the broad distribution of elastic intensity along  $T_1[\xi\xi 2\xi]$  and  $T_1[\xi\xi 0]$  and as shown in Fig. 2. In so far as this is true, the real phonon density of states will slightly differ from that shown in Fig. 4 by a stronger weighting of the phonons below the first singularity in Fig. 4, i.e., below 9 meV. Consequently,  $S_{\text{vib}}$  shifts to even higher values.

Furthermore, the strong damping questions the periodicity of certain lattice vibrations. This can be checked by measuring the phonon groups at equivalent but different points in reciprocal space. This has been done on the alloyed system  $\beta\text{-Zr}_{1-x}\text{Nb}_x$ ,<sup>16,17</sup> and strong violations of a one-phonon-scattering law, usually valid in all Brillouin zones, were found. However, only recent measurements on pure  $\gamma$ -La (the bcc phase of La) (Ref. 18) showed that

these effects are not due to alloying or the assumed coexistence of two phases,<sup>16,17</sup> but are generic to a lattice with strongly anharmonic interaction potentials. Similar effects are expected for  $\beta$ -Sc, but have not been looked for in the present study.

## CONCLUSION

We conclude that the phonon dispersion in  $\beta$ -Sc is dominated by a set of low-energy transverse phonons. Their eigenvectors are in the direction of the displacements needed for the transformation into the low-temperature  $\alpha$  phase and toward a hitherto unobserved  $\omega$  phase, thereby indicating low potential barriers for these displacive transitions. Most striking is the strong damping of these phonons with lifetimes at the zone boundary in the order of one vibrational period. The  $T_1[\xi\xi 2\xi]$  and  $T_1[\xi\xi 0]$  phonon branches are almost dispersionless, whereas perpendicular to these propagation directions the  $L_{\frac{2}{3}}(111)$  phonon is characterized by a narrow (but deep) minimum in the  $L[\xi\xi\xi]$  dispersion. In real space this means qualitatively that excitations propagate along [111] chains, whereas those perpendicular to [111] are to a certain extent localized. If a [111] chain vibrates along its chain direction, neighboring [111] chains do not follow this motion. Along [111] chains strong restoring forces are acting, whereas those perpendicular to [111] are weak.

The phonon dispersion of  $\beta$ -Ti very much resembles the one of  $\beta$ -Sc; i.e., the addition of a second  $d$  electron is not sufficient to hinder significantly the shearing motion of [111] chains relative to each other. The importance of increasing the  $d$ -electron density, causing an entanglement of this shearing motion, has been shown by frozen-phonon calculations<sup>19</sup> in the Zr-Nb-Mo system. Going from group IV to V, the  $d$ -electron density changes from  $4d^2$  (Zr) to  $4d^4$  (Nb), resulting in a drastic change of the lattice dynamics: Frequencies increase, and damping vanishes.

TABLE IV. Debye temperature  $\Theta_D$ , mean-square displacement  $\langle u_i^2 \rangle$ , lattice entropy  $S_{\text{vib}}$ , and the elastic constants  $C_{ij}$  for  $\beta$ -Sc at 1673 K. For comparison,  $\Theta_D = 310.5$  K for  $\alpha$ -Sc at room temperature (Ref. 8).

$T$ (K)	$\Theta_D$ (K)	$S_{\text{vib}}$ ( $k_B/\text{atom}$ )	$\langle u_x^2 \rangle$ ( $\text{\AA}^2$ )	$C_{11}$	$C_{12}$ ( $10^{10}$ N/m <sup>2</sup> )	$C_{44}$	$C'$
1673	243	9.64	0.092	7.33	6.05	2.64	0.64

This study will now enable one to compare more quantitatively the lattice dynamical behavior of the  $3d$  transition metals which solidify in the bcc structure. Special attention will be given to theories which explain the dynamical features of these metals with changing  $d$ -electron density, causing a characteristic directional bonding.

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<sup>1</sup>La is an exception and shows the unusual phase sequence dhcp-fcc-bcc.

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<sup>10</sup>It may be argued that the smeared intensity distribution observed along  $T_1[\xi\xi 2\xi]$  is caused by insufficient resolution in  $Q$  space. This has been ruled out by various tests on  $\beta$ -Zr, which shows similar broadened phonons with drastically re-

duced horizontal ( $10'$ ) and alternatively reduced vertical ( $\sim 1.1^\circ$ ) resolution. No change in line shape due to the reduced divergence has been observed.

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