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Lattice dynamics of solid n- and y-N, crystals at various pressures

Eduardo Huler
Department of Inorganic and Physical Chemsitry, Soreq Nuclear Research Centre, Yavne,

LATTICE DYNAMICS OF SOLID n- AND y-N, CRYSTALS... where Do„'o„. denote intramolecular atom-atom dis-

5880 g UNQEB

&I& D&S&ERSON CURVES

0
Q

0

C4 XXX X X X XX 0 X

~0pf
Q
S
~pH 'U

~ %

0

O
0
Of

o&

~0A
Q
0

'Q

0
O

cd 0

C

Dispersion cur for &-

a

and y-N& were ca

culated solving the dynamica equauations at 3o

LATTICE DYNAMICS OF SOLID a- AND y-Ng CRYSTA LS...

TABLE I. Comparison between calculated and measured inelastic-neutron-scattering (Ref. 15) lattice frequencies at high-symmetry points in the Brillouin zone. The values in parenthesis correspond to the optical measurements (Refs. 13-16). Values given in cm ~.

Calc.

I' Point

Obs.

M Point

Obs.

R Point

Calc.

X Point

Obs,

69. 5
47. 5
51, 8
47. 0
43. 7
38. 5
34, 5

69.60 (70. 0)
60. 0 (60. 0)
54. 20

48. 56 (36. 0)
46. 92

36.42 (36.0)
32. 37 (31.5)

61.2

53.7
42. 9
34. 7
24. 6

62, 7

55. 0
46. 9
38.0
27. 9

68.4

42. 0
40. 8
32. 9
32. 2

68.

IOQ

~

W

CQ

cf

CPo

QNQ

Gh

cj Q

'aC

cl Q
c5o

bSo
ChO

u

Q

oo

Ia

oQ

Cb
Cg
II
II

f~1

I

I

LIJ

II

.i

o

S
cf

II

cd

cjSo6

~

WQ0o
'U
cd

II

gf

cdNQ

q3o

cfQ

~

WN

o

o

c8QQ

(

(UJ0) AJUBilbp)g

Q

NS6

cd

c8Q

'QQl

'e t+4

o 0

cd
V

CDo

~

a

MQ

Qe ee o

Q eel m
Ch

~

I

'I

C3

~l

ll

n- AND y-N3 CRYSTA LS...

6xiO '

I

'

I

'

I

0-N2 (aj
V = 27.2cm5

4xlO '
0-N2

V = 24.I cd

I, I I. I

(b)

C3

D
U)

VP

2xIO

I xIO — ~ ~

I

Y- N2
V = 24.lcm

I

I
I

I

5xlO

0
0 20 00 60 80 IOO l20

FIG. 5. Density of states of &- and y-N2. (a) O'-N2 at V=27. 2 cm3; Q) O.'-N2 at V=24. 1 cm3; (c) y-N2 at V =24. 1 cms.

density-of-lattice-states function D(v) for n-Nz and y-Nz at various volumes. The standard meth-od was used for a cubic a phase while suitable
modifications were introduced into the BZ sampling
scheme for treating the tetragonal y phase. Stan-
dard channel widths of 0.25 cm ' were employed.
The convergence properties of the calculated den-
sity of states were examined by requiring that the
calculated nth5 8.77 Tf 91.81 615.45 teTd (')Tj ET BT /Xi5 2.48 Td 05 615.8 Td (the)TjTd (channel)Tj ET BT f 254.08 615.56 Td (72.83 604.63 Td (ca7Tj ET

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8'"'=(h/k)[-'(n+3)(uP)]'~", n &-3 nvO. (16)
GD"' is the cutoff temperature of a Debye

LATTICE DYNAMICS OZ SOLID n- AND y-N, CRYSTALS... sass

periments the most common choice of Domb and Salter e» =(~) is employed.
Experimental determination of 8~ for the n phase are: 68 'K at T= 20 K, 73 'K at'4 10 K and 80.6' at the lowest temperature measured T=4. 2 = 4. 2 'K. ' Our calculation yields 8~ = 84. 4 K at
the unit-cell volume corresponding to equilibrium at 7. = 0 K in good agreement with the value of
Bagatoskii et al. Using the linear expansion co-
efficient determined experimentally by Bolz et
al.,

the calculated Q~ at the unit-cell volume cor-
responding to 20 'K is 75. 3 'K, in reasonable agreement with the experimental data. '
Schuch and Mills' have estimated OD in comput-
ing the experimental Debye-Wailer factor for y-N2, using the de Boer reduced equation of state' as an interpolation scheme, obtaining OD = 94 'K. Our calculated value of 125.0 'K is considerably higher and provides a better approximation. A lower Debye-Wailer factor is thus predicted by the pres-ent calculation. It should be noted that our calcu-lation of the volume dependence of the Debye tem-perature QD(V) predicts similar values for the n and the y phases at the same volume, in agree-ment with the approximation made by Raich'~ in calculating n-to-y phase transition.

V. THERMAL EXPANSION

The density of states D(~) is used to compute the
thermal-expansion coefficient of n-N~. This is
done by minimizing the total crystal free

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a
E
0

4)
O

CL 2

0 20 30 40 50

V('K)
FIG. 9. Heat

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thermal-expansioGER

12 LA TT ICE DYNAMICS OF SO LID n- AND y-N~ CBYSTA I S... 5889

35M. I. Bagatoskii, V. A. Kucheryavy, V. G. Manzhelii,
and V. A. Popov, Phys. Status