independent components of **C** reduce from 108 to 48, which was the number obtained for the tensor **b** in the rotation-gradient theory. However, if we were to take into account the further restrictions implied by the relation (3.11) the number of independent components of **C** (or **Ĉ**) will be further reduced. A detailed analysis of all the constraints on **C** shows that only the six components C_{11223}, C_{11332}, C_{11132}, C_{22331}, C_{22231} and C_{33231} are independent. The other non-vanishing components are

$$C_{11232} = -C_{22131} = -2C_{13122} = 2C_{23121} = -\tfrac{1}{2}C_{11223}$$

$$C_{11233} = 2C_{23131} = -C_{33121} = -2C_{13123} = -\tfrac{1}{2}C_{11332}$$

$$C_{11123} = -2C_{13121} = -C_{11132}$$

$$C_{22133} = -C_{33122} = -2C_{23132} = 2C_{23123} = -\tfrac{1}{2}C_{22331}$$

$$C_{22123} = -2C_{23122} = -C_{22231}$$

$$C_{33132} = -2C_{23133} = -C_{33231}$$

and those related to the above by the intrinsic symmetry relation (3.3). It follows from the relations (3.21), (3.17), (3.10) and (2.8) (with the identification **d** = **Ĉ**) that the activity tensor **b** of the rotation-gradient theory which conforms to the restrictions from considerations of the total energy has only six non-vanishing independent components [as against 48 reported earlier (Bhagwat & Subramanian, 1986)] for the triclinic system and is related to the tensor **G** by the equation

$$b_{ijkp} = \tfrac{2}{3}[\, G_{pikj} - \delta_{pj}G_{qikq} + e_{lmp}e_{ikq}G_{qjml}\,].$$

The quantities $[b_{1331} + b_{2332}]$ and G_{3333} which govern the angle of rotation of a plane-polarized acoustic wave in the two descriptions respectively turn out to be proportional to the component C_{33231}. This shows that even this restricted tensor **b** will lead to acoustical activity in all those crystal classes which were found acoustically active in either of the two earlier descriptions. In other words, the restricted theory still retains the essential ingredients of the general theory as far as the explanation of acoustical activity is concerned.

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On the Deficiencies of the Anharmonic One-Particle Potential Model

BY HOLGER LÜDERS AND ELISABETH ROSSMANITH

Mineralogisch-Petrographisches Institut der Universität Hamburg, D-2000 Hamburg 13, Grindelallee 48, Federal Republic of Germany

Abstract

The temperature factors of Cd and Zn for $h00$ reflexions calculated by numerical Fourier transformation are compared with the temperature factors determined with the help of series expansion of the anharmonic term of the probability density function (p.d.f.). The anharmonic parameters used have been derived by least-squares fit of measured Bragg intensities in the framework of the anharmonic one-particle potential (OPP) model. For Cd a deviation of up to 7% is found for the results obtained for the symmetric part and up to 50% for the antisymmetric part of the temperature factor. It is shown that numerical Fourier transformation of the p.d.f., using the anharmonic parameters given in the literature for Zn, is not always possible, because the p.d.f. is divergent for some of these parameters.

Theory

In this paper the anharmonic one-particle potential (OPP) formalism for the hexagonal structures Zn and Cd given by Merisalo & Larsen (1977) (hereafter ML77) was used. To reduce the number of degrees of freedom of the potential from about 10^{23} to 3, the potential experienced by an atom in the OPP model is assumed to be independent of the motion of all other atoms of the lattice (Willis & Pryor, 1975).

To allow for anharmonic motion the potential is expanded into a series up to fourth order. Because of the $\bar{6}m2$ site symmetry of the Zn atom in the h.c.p. lattice the number of third-order parameters reduces to one and the number of fourth-order parameters reduces to three, and the potential is given by (ML77)

$$V(\mathbf{u}) = V_0 + u^2(\alpha_{20}K_{20} + \beta_{00}) + u^3\alpha_{33}K_{33}$$
$$+ u^4(\alpha_{40}K_{40} + \beta_{20}K_{20} + \gamma_{00}). \quad (1)$$

V_0, α_{ij}, β_{ij}, γ_{ij} are parameters of the potential. $\mathbf{u}$ is the vector of displacement from the equilibrium position with $u^2 = u_1^2 + u_2^2 + u_3^2$ and u_i are the components of $\mathbf{u}$ parallel to [210], [010], [001] respectively. The K_{ij} are symmetry-adapted harmonics given by

$$K_{20} = 0 \cdot 5(3u_3^2 - u^2)/u^2 \quad (2a)$$

$$K_{33} = (u_1^3 - 3u_1u_2^2)/u^3 \quad (2b)$$

$$K_{40} = 0 \cdot 125(35u_3^4 - 30u_3^2u^2 + 3u^4)/u^4. \quad (2c)$$

In the classical regime the probability density function (p.d.f.) of an atom, defined as the probability of finding the atom in the volume element d^3u when it is displaced by $\mathbf{u}$, is obtained from the potential according to the Boltzmann distribution

$$\text{p.d.f.} = \exp\left[-V(\mathbf{u})/(kT)\right]/Z \quad (3)$$

with

$$Z = \int\int\int_{-\infty}^{\infty} \exp\left[-V(\mathbf{u})/(kT)\right] du_1\, du_2\, du_3, \quad (4)$$

where k is the Boltzmann constant, T is the absolute temperature and Z is the partition function.

The temperature factor is the Fourier transform of (3) (Willis, 1969):

$$T(q) = \int\int\int_{-\infty}^{\infty} \text{p.d.f.} \times \exp(i\mathbf{q}\mathbf{u})\, du_1\, du_2\, du_3, \quad (5)$$

where q is the scattering vector.

Because the Fourier transform of the anharmonic p.d.f. given in (3) cannot be written as a closed algebraic expression, the anharmonic part of the p.d.f. is expanded into a series (Willis, 1969) to make analytical integration, $i.e.$ Fourier transformation, possible.

$$\text{p.d.f.} = \{\exp\left[-V(\mathbf{u})_{\text{harm}}/(kT)\right]$$
$$\times [1 - V(\mathbf{u})_{\text{anharm}}/(kT) + \dots]\}/Z'. \quad (6)$$

$V(\mathbf{u})_{\text{harm}}$ and $V(\mathbf{u})_{\text{anharm}}$ are the harmonic and the anharmonic part of the potential given in (1), and Z' is the corresponding partition function.

The analytical expression for the temperature factor, given by the Fourier transform of (6), is called $T(q)_{\text{series}}$ in the following, in contrast to $T(q)_{\text{num}}$, which is evaluated by numerical integration.

To make numerical evaluation of the Fourier transform (5) possible, the integration is confined to the finite range occupied by the atom (Matsubara, 1975).

For the evaluation of $T(q)_{\text{num}}$, the p.d.f. was divided into its even and odd parts p.d.f.$_{\text{even}}$ and p.d.f.$_{\text{odd}}$.

$$\text{p.d.f.}_{\text{even}} = \{\exp\left[-u^2(\alpha_{20}K_{20} + \beta_{00})/(kT)\right.$$
$$\left.- u^4(\alpha_{40}K_{40} + \beta_{20}K_{20} + \gamma_{00})/(kT)\right]$$
$$\times \cosh\left[(u^3\alpha_{33}K_{33})/(kT)\right]\}/Z'' \quad (7a)$$

$$\text{p.d.f.}_{\text{odd}} = \{\exp\left[-u^2(\alpha_{20}K_{20} + \beta_{00})/(kT)\right.$$
$$\left.- u^4(\alpha_{40}K_{40} + \beta_{20}K_{20} + \gamma_{00})/(kT)\right]$$
$$\times (-1)\sinh\left[(u^3\alpha_{33}K_{33})/(kT)\right]\}/Z'' \quad (7b)$$

with

$$Z'' = \int\int\int_{-u_l}^{u_l} \exp\left[-V(\mathbf{u})/(kT)\right] du_1\, du_2\, du_3. \quad (7c)$$

With the approximations

$$T_c(q)_{\text{num}} = \int\int\int_{-u_l}^{u_l} \text{p.d.f.}_{\text{even}} \cos(\mathbf{q}\mathbf{u})\, du_1\, du_2\, du_3 \quad (8a)$$

$$T_a(q)_{\text{num}} = \int\int\int_{-u_l}^{u_l} \text{p.d.f.}_{\text{odd}}\, i \sin(\mathbf{q}\mathbf{u})\, du_1\, du_2\, du_3 \quad (8b)$$

where $T_c(q)$ is the centrosymmetric (real) and $T_a(q)$ is the antisymmetric (imaginary) part of the temperature factor, with $i = \sqrt{(-1)}$, the corresponding temperature factor $T(q)_{\text{num}}$ is given by

$$T(q)_{\text{num}} = [T_c^2(q)_{\text{num}} + T_a^2(q)_{\text{num}}]^{1/2}. \quad (8c)$$

u_l represents the limits of integration, introduced under the assumption that a physically meaningful p.d.f. has to be convergent and therefore can be approximated by zero outside a finite range of $\mathbf{u}$.

Comparison of $T(q)_{\text{num}}$ and $T(q)_{\text{series}}$ for Cd and Zn

With the Fourier transform of (6) given by ML77 [formula (6) in their paper] the temperature parameters α_{ij}, β_{ij} and γ_{ij} can be determined by a least-squares fit of calculated to observed intensity data. For the different models of refinement used by several authors, different sets of parameters were obtained. A collection of these parameters, a description of the models used and a detailed discussion of the reliability of the temperature parameters are given by Rossmanith (1984). Parameters which are used in this

Table 1. *Anharmonic temperature parameters of* Zn *and* Cd *used in this paper*

Reference		α_{20} $(10^{-19}$ J Å$^{-2})$	β_{00} $(10^{-19}$ J Å$^{-2})$	α_{33} $(10^{-19}$ J Å$^{-3})$	α_{40} $(10^{-19}$ J Å$^{-4})$	β_{20} $(10^{-19}$ J Å$^{-4})$	γ_{00} $(10^{-19}$ J Å$^{-4})$	Radiation
Rossmanith	Cd	−0·6057 (10)	1·1293 (10)	0·079 (99)	0·415 (133)	−2·008 (154)	1·843 (99)	Mo $K\alpha$
Merisalo & Larsen (1979), model 3	Zn	−1·109 (10)	1·841 (10)	−1·80 (30)	0·25 (28)	7·36 (28)	−6·27 (14)	Neutrons

paper are listed in Table 1. The parameters for Cd were evaluated without extinction correction, using the Bragg intensities of Rossmanith (1984) in a $(\sin \theta)/\lambda$ range from 0·41 to 0·79 Å^{-1}.

For Zn the parameters of model 3 given by Merisalo & Larsen (1979) are tabulated. The radiations used in the measurements are also given in Table 1.
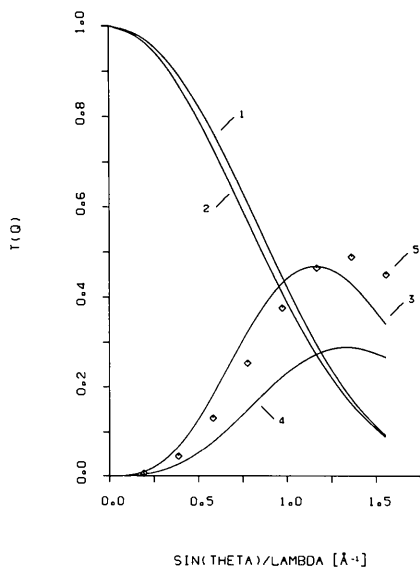

SIN(THETA)/LAMBDA [Å⁻¹]

Fig. 1. The temperature factors of *h*00 reflexions for Cd in a $(\sin \theta)/\lambda$ range up to 1·55 Å^{-1}. $T_a(q)$ has to be multiplied by 0·01. Curve 1: $T_c(q)_{\text{series}}$; 2: $T_c(q)_{\text{num}}$; 3: $T_a(q)_{\text{series}}$; 4: $T_a(q)_{\text{num}}$; and 5: $T_a(q)_{\text{num}}$ with $\alpha'_{33} = 1·7\alpha_{33} = 0·1343 \times 10^{-19}$ J Å^{-3}.
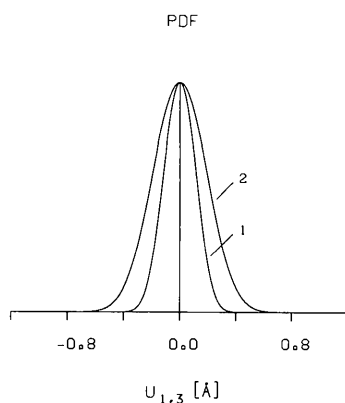
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$U_{1,3}$ [Å]

Fig. 2. The p.d.f. [formula (3)] for Cd. Curve 1 in the u_1 direction, 2 in the u_3 direction. u_i given in Å.

Table 2. *The partition function* Z'' *evaluated with the anharmonic parameters for* Zn, *for increasing values of* u_l

u_l (Å)	Z''
±0·05	0·0009
±0·10	0·0053
±0·15	0·0120
±0·20	0·0185
±0·25	0·0241
±0·30	0·0315
±0·35	0·2567
±0·40	4023·6786

(*a*) Cd

In Fig. 1 the results for $T_{c,a}(q)_{\text{num}}$ and $T_{c,a}(q)_{\text{series}}$, both calculated with the parameters for Cd in Table 1, are shown. Fig. 2 represents the p.d.f. [formula (3)] used in the evaluation of $T_{c,a}(q)_{\text{num}}$. The $T_{c,a}(q)_{\text{num}}$ were calculated repeatedly with increasing values for the u_l. The range of integration was assumed to be appropriate when, within the limits of computational precision (64 bits per real variable), identical results were obtained for successive calculations.

The values of u_l in the u_1, u_2 and u_3 directions never exceed 1·2 Å, whereas the p.d.f. becomes negligibly small for u values greater than 0·4 Å in the u_1 and u_2 directions and 0·7 Å in the u_3 direction, as can be seen in Fig. 2.

In the region of $(\sin \theta)/\lambda$ between 0·4 and 1·3 Å^{-1} (Fig. 1), which is essential for temperature parameter determination, $T_{c,a}(q)_{\text{num}}$ and $T_{c,a}(q)_{\text{series}}$ differ considerably, $T_{c,a}(q)_{\text{num}}$ being smaller for all $(\sin \theta)/\lambda$ values than $T_{c,a}(q)_{\text{series}}$. The deviation is more remarkable for $T_a(q)$ (up to 50%) than for $T_c(q)$ (up to 7%). The series expansion (6) underestimates α_{33}, as can be seen from Fig. 1, where $T_a(q)_{\text{num}}$, calculated with a third-order parameter α'_{33} ($\alpha'_{33} = 1·7\alpha_{33} = 0·1343 \times 10^{-19}$ J Å^{-3}), is also given.

(*b*) Zn

For the calculation of $T(q)_{\text{num}}$ with the parameters for Zn given in Table 1 the same procedure as for Cd was used. But, as can be seen from Table 2, the partition function [formula (7*c*)] does not converge with increasing range of integration. Inspection of the p.d.f. used in the calculations explains this behaviour. As can be seen in curve 1 of Fig. 3, the non-standardized p.d.f.$_{\text{even}}$ [numerator in (7*a*)] cannot be approximated by zero in the surroundings of the equilibrium position of the atom. The p.d.f. given

in (3) is physically meaningless when it is used with the parameters for Zn.

The p.d.f. defined by (6), whose Fourier transform is $T(q)_{series}$, is convergent (Fig. 3, curve 2) and therefore a useful p.d.f.

The one-particle potential

If one starts from formula (3) the one-particle potential can be calculated as

$$V(\mathbf{u}) = -kT \ln (\text{p.d.f.} \times Z) \qquad (9)$$

(Zucker & Schulz, 1982).

Insertion of the p.d.f. [Fig. 3, curve 2; formula (6)] in (9) results·in the potential presented in curve 2 of Fig. 4, whereas curve 1 of Fig. 4 shows for comparison the potential given by (1). For both figures the parameters for Zn of Table 1 were used. In the region $|\mathbf{u}| = 3\langle u^2 \rangle^{1/2}$ (three times the root mean square displacement, r.m.s.d., with $\langle u_{1,2}^2 \rangle^{1/2} = 0 \cdot 1063$ Å), where the p.d.f. is significantly greater than zero, the
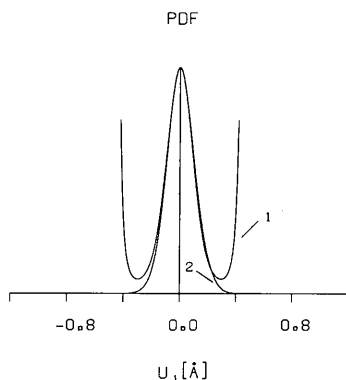
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Fig. 3. The p.d.f. of Zn. Curve 1: the non-standardized p.d.f.$_{even}$ [formula (7a)] in the u_1 direction, u_i given in Å. Curve 2: p.d.f. defined in formula (6) in the u_1 direction, u_1 given in Å.
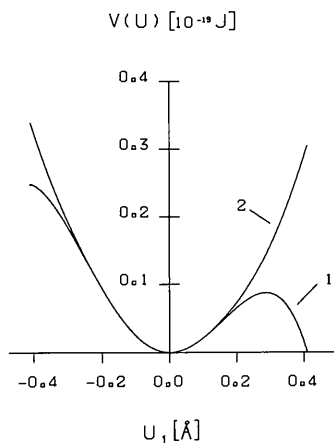
$V(U)$ $[10^{-19} \text{ J}]$

Fig. 4. The potential of Zn in the u_1 direction (Å). Curve 1: formula (1); curve 2: formula (9). u_1 given in Å.

Table 3. *The potentials $V_1(\mathbf{u})$, $V_2(\mathbf{u})$, the values of $V(\mathbf{u})_{anharm}/(kT)$ and the errors E for one, two and three times the r.m.s.d.*

	u_x (Å)	$V_1(\mathbf{u})^*$	$V_2(\mathbf{u})^*$	$V(\mathbf{u})_{anharm}/(kT)$	$E(\%)$
Cd	−0·3480†	0·2141	0·5073	0·9997	99·93
	−0·2324	0·0851	0·0860	0·1908	2·07
	−0·1162	0·0198	0·0198	0·0104	0·01
	0·1162	0·0200	0·0200	0·0165	0·01
	0·2324	0·0871	0·0885	0·2395	3·37
	0·3348†	0·2012	0·4571	0·9993	99·81
Zn	−0·3189	0·2001	0·2140	−1·0698	28·99
	−0·2126	0·1054	0·1055	−0·0697	0·23
	−0·1063	0·0280	0·0280	0·0222	0·02
	0·1063	0·0236	0·0238	−0·0840	0·33
	0·2126	0·0708	0·0817	−0·9193	23·46
	0·3189	0·0833	0·1786	−3·9371	90·37

* $V_1(\mathbf{u})$: Potential calculated with formula (1), $V_2(\mathbf{u})$: potential calculated with formula (9), both multiplied by 10^{-19} J.

† Maximal possible value for $u_x < 3$ times r.m.s.d. (see text).

two potentials (Fig. 4) differ appreciably. It has to be concluded that the potential of curve 2 does not approximate the potential of curve 1 and *vice versa*. Therefore, in the case of Zn, the anharmonic parameters α_{33}, α_{40}, β_{20} and γ_{00}, evaluated from a truncation of (3) by a least-squares fit of calculated and measured Bragg intensities, are no longer identical with the parameters of the potential in (1).

Discussion

In the OPP model of Willis (1969) it is assumed that the anharmonic potential $V(\mathbf{u})_{anharm}$ is much smaller than kT, and that therefore $[V(\mathbf{u})_{anharm}/(kT)]^2$ and higher-order terms are negligible in (6). But for large values of $\mathbf{u}$, $V(\mathbf{u})_{anharm}$ is always larger than kT. However, in a real crystal the probability that $\mathbf{u}$ exceeds a certain limiting value can be approximated by zero. Tanaka & Marumo (1983) therefore proposed to judge the validity of the Willis treatment of anharmonicity from the $V(\mathbf{u})_{anharm}/(kT)$ value at a u value equal to the r.m.s.d. of the atom which is calculated from the harmonic temperature factor. In Table 3 the potentials $V(\mathbf{u})$ defined in (1) and (9) are given together with $V(\mathbf{u})_{anharm}/(kT)$ for $u_1 = \pm\langle u_x^2 \rangle^{1/2}$, $\pm 2\langle u_x^2 \rangle^{1/2}$ and $\pm 3\langle u_x^2 \rangle^{1/2}$, where $\langle u_x^2 \rangle^{1/2}$ is the r.m.s.d. in the basal plane of the hexagonal crystals of Zn (given by Merisalo & Larsen, 1979) and Cd. The percentage error E of the approximation $\exp(x) \simeq 1 + x$, with $x = -V(\mathbf{u})_{anharm}/kT$, is tabulated in the fifth column of Table 3.

In the case of Cd the error of the approximation for $u_1 =$ one r.m.s.d. is much less than 1%, reaching up to about 100% for $u_1 \lesssim$ three times the r.m.s.d. For greater or smaller values of u than those given in Table 3, the p.d.f. defined in (6) is very small but negative and the potential given by (9) is not defined.

In the case of Zn the error reaches about 29% in the negative u_1 direction and 90% in the positive u_1 direction.

Therefore, it has to be concluded that judgement of the validity of the approximation at u_1 equal to one r.m.s.d. is not sufficient. An interval of at least three times the r.m.s.d. should be taken into consideration.

If large anharmonic effects are supposed, even greater regions in **u** have to be considered, because of the deformation of the normal distribution of the harmonic p.d.f.

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Determination of Structure-Factor Phase Invariants and Effective Structure Factors in Non-centrosymmetric Crystals

BY KNUT MARTHINSEN* AND RAGNVALD HØIER

Department of Physics and Mathematics, University of Trondheim-NTH, N-7034 Trondheim, Norway

Abstract

Many-beam diffraction effects in non-centrosymmetric crystals have been studied with emphasis on three-beam interactions and determination of three-phase structure invariants in electron diffraction experiments. The effective structure factor has been determined both by numerical many-beam calculations and from the second Bethe approximation. The dependence of this factor on the phase invariant, the excitation errors and the magnitude of the structure factors involved has been discussed in detail. From the values of the effective structure factors at symmetrical positions on each side of a three-beam condition an asymmetry ratio is introduced. By a comparison of the observed variation in this ratio with theoretical profiles, it has been shown that the magnitude of three-phase invariants can be determined in the non-centrosymmetric case. This method may in principle be applied in any type of electron or X-ray three-beam experiments where variations in the effective structure factor are projected out. An example from electron channelling patterns is given.

Introduction

The structure-factor phase problem is central in all crystallographic diffraction studies, and various methods are used to handle it. In X-ray structure determination using direct methods phases are usually estimated with some probability by statistical methods from relations between structure-factor

amplitudes (*e.g.* Woolfson, 1987). One direct way, however, to solve the problem is to utilize the intensity anomalies observed in dynamical many-beam diffraction experiments. Here additional information is available compared with standard experiments. This concerns in principle both the magnitudes of the structure factors and the three-phase structure invariants.

In many-beam investigations a perturbed two-beam, or two-Bloch-wave, point of view has often proved to be successful. On this basis the effective structure factor has been introduced, and a theoretical background for obtaining structure-factor phase information has been established. It is clear that three-phase invariants, in principle, can be determined from any type of electron or X-ray three-beam experiment where the effective structure factor, *i.e.* the effective dispersion surface gap width, is projected out. In practice this possibility is now well established for the centrosymmetric case.

Dependence of the observed intensity anomalies on the various parameters in mainly centrosymmetric crystals has been discussed in non-systematic many-beam electron diffraction cases by, for example, Kambe (1957), Gjønnes & Høier (1971), Gjønnes (1981) and Marthinsen & Høier (1986). The X-ray case has been discussed by Post (1979, 1983), Chapman, Yoder & Colella (1981), Marthinsen (1981), Thorkildsen & Mo (1982), Chang (1982, 1986), Juretschke (1982, 1986), Hümmer & Billy (1982, 1986), Høier & Marthinsen (1983), Thorkildsen (1987) and Marthinsen & Høier (1987).

In the present studies we shall focus on the determination of effective structure factors and a new method

* Present address: SINTEF, Division of Applied Physics, N-7034 Trondheim, Norway.