

APPENDIX 2

Atoms in the 6D MgCu₂ rhombohedron

Let us assume that the acute rhombohedron ($\alpha = 63.43^\circ$) of the 3D Penrose tiling has a similar structure to the 3D MgCu₂ rhombohedron ($\alpha = 60^\circ$) which has two atoms at $\pm(\frac{3}{8}\frac{3}{8}\frac{3}{8})$ in addition to those at the vertices and the centres of edges. This acute rhombohedron can have 20 different orientations. But one half of them are in the opposite direction to the other half, so that only ten independent orientations exist. Let the basis vectors be \mathbf{q}_i , \mathbf{q}_j and \mathbf{q}_k , where the set i, j, k may have the values

$$(126), (236), (346), (456), (156),$$

$$(1\bar{2}\bar{4}), (2\bar{3}\bar{4}), (\bar{1}3\bar{4}), (\bar{2}5\bar{4}), (\bar{1}\bar{3}5).$$

The coordinates of these 20 atoms inside the rhombohedron are

$$\pm(\frac{3}{8}\frac{3}{8}00\frac{3}{8}), \pm(0\frac{3}{8}\frac{3}{8}00\frac{3}{8}), \pm(00\frac{3}{8}\frac{3}{8}0\frac{3}{8}),$$

$$\pm(000\frac{3}{8}\frac{3}{8}\frac{3}{8}), \pm(\frac{3}{8}000\frac{3}{8}\frac{3}{8}), \pm(\frac{3}{8}\frac{3}{8}0\bar{3}\frac{3}{8}),$$

$$\pm(0\frac{3}{8}\frac{3}{8}0\bar{3}\frac{3}{8}), \pm(\frac{3}{8}0\frac{3}{8}\bar{3}\frac{3}{8}), \pm(0\bar{3}\frac{3}{8}\frac{3}{8}\frac{3}{8}),$$

$$\pm(\frac{3}{8}0\bar{3}\frac{3}{8}\frac{3}{8}).$$

Together with the atom at the origin and six more atoms on the centres of the edges with coordinates $(\frac{1}{2}0000) \odot$, there are altogether 27 atoms. Since the \mathbf{q}_i are the projection of \mathbf{b}_i , these 27 atoms can be considered as projected from a 6D unit cell. By projecting such a 6D unit cell onto a 3D hyperplane, the atomic positions in the icosahedral quasicrystal can be obtained.

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Debye–Waller Coefficient of Nb by the Elastic Neutron Diffraction Method

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Abstract

The Debye–Waller exponent B and the Debye temperature Θ for niobium have been determined at room temperature by the elastic neutron diffraction method using a triple-axis neutron spectrometer. The contribution of TDS to the diffraction peaks was found to be negligible. The value of B thus found was $0.55(5) \text{ \AA}^2$. The Debye temperature Θ was

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262 (12) K. The results are compared with values obtained by other techniques.

Introduction

From a diffraction experiment one could, in principle, obtain information about lattice-dynamical properties such as the mean square displacement of an atom and the Debye temperature of the material.

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In the present experiment, the powder neutron diffraction method has been employed and from the measurement of integrated intensities of several Bragg reflections of niobium, the Debye-Waller factor, the Debye temperature and the mean square amplitude have been determined. Similar measurements were carried out by Linkoaho (1971) using X-rays. Sharp (1969) and Powell, Martel & Woods (1977) determined the Debye temperature of niobium from the measured phonon density of states using the inelastic neutron scattering technique and Grimvall & Grimvall (1968) determined the Debye temperature using the inelastic neutron scattering data of Nakagawa & Woods (1963). However, there is a considerable discrepancy among their results. Since no measurements are available using the neutron diffraction method we took up these experiments. These data are of interest to the IUCr project on the compilation of temperature factors for cubic elements (International Union of Crystallography, 1985).

Theory

The integrated intensity of a Bragg reflection depends on the specimen temperature through the Debye-Waller factor, $\exp(-2M)$, which is related to the Debye-Waller parameter B by

$$M = B (\sin^2 \theta) / \lambda^2,$$

where

$$B = 8\pi^2 \overline{u^2} / 3.$$

Here $\overline{u^2}$ is the mean square atomic displacement perpendicular to the reflecting plane, θ is the Bragg angle and λ is the wavelength of radiation employed.

The Debye-Waller parameter B is obtained from the slope of the line given by

$$\ln (F_o / F_c) = \text{constant} - B(\sin^2 \theta) / \lambda^2,$$

where F_o is the observed structure factor and F_c the calculated structure factor.

In the Debye approximation

$$B = (6h^2 / mk)(T / \Theta^2) [\varphi(x) + x/4]$$

where h is Planck's constant, k is Boltzmann's constant, m is the atomic mass, T is the temperature of measurement, Θ is the Debye temperature and $\varphi(x)$ is the Debye function where $x = \Theta / T$.

Experimental procedure

A triple-axis neutron spectrometer was used in the elastic diffraction mode for the measurement of the

Table 1. Observed and calculated structure factors and the TDS correction for Nb at room temperature

<i>hkl</i>	F_o	F_c	TDS(%)
110	14.37	14.42	0.03
200	14.43	14.07	0.08
211	13.77	13.72	0.12
220	13.39	13.39	0.17
310	12.60	13.06	0.21

Bragg intensities. (Beg, Aslam, Butt, Khan & Rolandson, 1974). Niobium powder (325 mesh, purity 99.9%) was packed in a moisture-tight vanadium container. (220) planes of a copper single crystal were used as monochromator and (200) planes of a pyrolytic graphite crystal as the analyser. The neutron wavelength employed was 1.175 Å. The Bragg peaks were scanned over a 2θ range of 75° and counts were noted at angular intervals of 0.20°. Peak intensities were corrected for the background defined by the wings of the peak. All measurements were made at room temperature (298 K).

The integrated intensities were corrected for thermal diffuse scattering (TDS) by the method described by Beg *et al.* (1974). The B value of niobium was computed by least-squares fitting of the data of five peaks. The TDS error varied from 0.03% for the 110 reflection to 0.2% for the 310 reflection. The correction to the B value due to TDS was thus found to be small and was within experimental errors.

Results and discussion

The least-squares fit to the experimental data yielded a value of $B = 0.55(5) \text{ \AA}^2$ corresponding to a Debye temperature of 262(12) K and a root mean square displacement of 0.145(6) Å.

Table 1 contains the values of the observed and calculated structure factors. The discrepancy factor R was 1.3%, indicating good agreement between the observed and the calculated structure factors.

In Table 2 the results of previous experimental and theoretical determinations of B values are summarized. In the present work using the powder neutron diffraction method, the value of $B = 0.55(5) \text{ \AA}^2$ agrees well with the previous X-ray and inelastic neutron scattering values which lie in the range 0.45 to 0.53 Å². The average B value determined from elastic-constant data is 0.54 Å², and the agreement between experimental and theoretical values is also good. The B value for Nb determined in the present experiment can be regarded as a reliable value.

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Table 2. Comparison of results for B values of Nb

B (Å ²)	Θ (K)	$(\overline{u^2})^{1/2}$ (Å)	Method	Reference
0.53	270	0.142	Inelastic neutron scattering data	Grimvall & Grimvall (1968)
0.45	285	0.131	Inelastic neutron scattering data	Sharp (1969)
0.50	279	0.138	Inelastic neutron scattering data	Powell, Martel & Woods (1977)
0.45 (2)	285 (5)	0.131 (1)	X-ray powder diffraction	Linkoaho & Rantavuori (1970)
0.45 (1)	284 (6)	0.134 (1)	X-ray powder diffraction	Linkoaho (1971)
0.52 (8)	260 (20)	0.140 (40)	X-ray powder diffraction (not corrected for TDS)	Korsunskii, Genkin & Vigdorichik (1977)
0.56	260	0.146	Elastic constant data	Padyukha & Chernyi (1966)
0.51	275	0.139	Elastic constant data	Jones, Moss & Rose (1969)
0.56	256	0.146	Elastic constant data	Gololobov, Mager, Mezhevich & Pan (1983)
0.49	281	0.136	Theoretical (model calculations)	Gupta (1985)
0.55 (5)	262 (12)	0.145 (6)	Elastic neutron powder diffraction	Present work

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A Multisolution Procedure via Tendentially Maximally Entropical Starting Sets

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Abstract

Large starting sets of random phases are in general inconsistent with positivity and atomicity of the electron density. A correct solution can be achieved from them because the tangent formula is a process which maximizes entropy under physical constraints involving the positivity and atomicity of electron density. Starting sets which are themselves tendentially maximally entropical can be created by associating phase shifts Δ , generated according to the von Mises distribution of each triplet phase, to some (from 50 to 300) triplet invariants. Then the phases generated via these perturbed triplets are samples of the phase population expected to be maximally entropical on

the basis of the prior information. Experimental tests show that the method may be a useful alternative to other conventional multisolution methods.

1. Introduction

Multisolution direct-methods computer programs are today a powerful tool for solving structures containing up to 70 or 80 atoms in the asymmetric unit. Various sets of phases, among which the correct solution is usually found, are produced by application of the tangent formula or similar techniques. The unknown phase values among the reflexions chosen to start the phase determination are usually represented by a magic-integer sequence (White & Woolfson,