Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 14 April 2009
Accepted 15 May 2009

Three new types of interpenetrating sphere packings

Heidrun Sowa

GZG, Abteilung Kristallographie, Georg-August-Universität Göttingen, Goldschmidtstrasse 1, D-37077 Göttingen, Germany. Correspondence e-mail: heidrun.sowa@geo.uni-goettingen.de

Three new types of homogeneous interpenetrating sphere packings are described. In the general position of space group *Ccce*, two sphere packings of type 3/10/*o*1 can be combined to form interpenetrating sphere packings of type $o[3/10/o1]^2$. The other two types of interpenetrating sphere packings show symmetry *Fddd*: two packings of type 3/10/*t*4 are intertwined in $o[3/10/t4]^2$ and three packings of type 3/4/*t*1 in $o[3/4/t1]^3$.

In a previous paper (Koch *et al.*, 2006) all homogeneous interpenetrating sphere-packing types that occur with highest symmetry in the cubic, hexagonal or tetragonal crystal families have been tabulated. It was assumed that there are no or at most very few additional types with orthorhombic, monoclinic or triclinic symmetry. In the course of deriving the sphere packings with orthorhombic symmetry, however, three new types were found: two congruent sphere packings interpenetrate each other in two cases and three in one case.

In the general position of space group *Ccce*, two orthorhombic sphere packings of type 3/10/*o*1 (symmetry *Pnnb* 8*e*; Koch & Fischer, 1995) may intertwine (*cf.* Fig. 1), forming interpenetrating sphere packings of type $o[3/10/o1]^2$ [generators: 2 $(0, y, 0)$, 2 $(\frac{1}{4}, \frac{1}{4}, z)$, $\overline{1}$ $(\frac{1}{4}, 0, \frac{1}{4})$]. The corresponding three-dimensional parameter range in *Ccce* does not contain interpenetrating packings with minimal density (*cf.* Koch *et al.*, 2005). The orthorhombic pattern of interpenetration (symbol *o-s*) has not been described before (*cf.* Koch *et al.*, 2006).

In $o[3/10/t4]^2$, two othorhombically deformed sphere packings of the tetragonal type 3/10/*t*4 (Fischer, 1991*a*, 2005) are combined (*cf.* Fig. 2). This type occurs with four degrees of freedom in the general position of space group *Fddd* [generators: 2 $(\frac{1}{4}, y, \frac{1}{4})$, *d* $(x, y, \frac{3}{8})$]. It has only a very small parameter range and also does not constitute a configuration with minimal density. The individual packings have symmetry *Fdd*2 16*b*. The pattern *o-b* of interpenetration has already been observed. It corresponds to a combination of two orthorhombically distorted diamond configurations. Interpenetration of two sphere packings of type 3/10/*t*4, but with tetragonal symmetry, is also possible (*cf.* Koch *et al.*, 2006) in the general positions of $P4_22_12$ (type $t[3/10/t4]^2_{\rm I}$) and of $I\overline{4}2d$ (type $t[3/10/t4]^2_{\rm II}$).

Furthermore, in the general position of space group *Fddd*, three sphere packings of the tetragonal type 3/4/*t*1 (Fischer, 1991*b*, 2005) may be intertwined in two different ways, forming interpenetrating sphere packings of the types $t[3/4/t1]^3$ and $o[3/4/t1]^3$. In both cases, the symmetry group of an individual packing is an isomorphic subgroup of *Fddd* with triplication of one of the lattice parameters, and the parameter region shows three degrees of freedom. Interpenetrating sphere packings of type $t[3/4/t1]^3$ [generators: $\overline{1}$ $(-\frac{1}{8}, \frac{1}{8}, \frac{3}{8})$, 2 $(\frac{1}{4}, \frac{1}{4}, z)$, 2 $(\frac{1}{4}, y, \frac{1}{4})$] have tetragonal inherent symmetry, namely $I4_1/amd$ 16*h*, and may be orthorhombically distorted in the general position of *Fddd* (*cf.* Koch *et al.*, 2006), whereas the inherent symmetry of type $o[3/4/t1]^3$ [generators: $\overline{1}(-\frac{1}{8}, \frac{1}{8}, \frac{3}{8})$, 2 $(\frac{1}{4}, \frac{1}{4}, z)$, 2 $(x, \frac{1}{4}, \frac{1}{4})$] is orthorhombic. Both types show the same pattern of interpenetration, *o-m*, and have the same value for their minimal density, namely $\rho = 0.34665$, *i.e.*

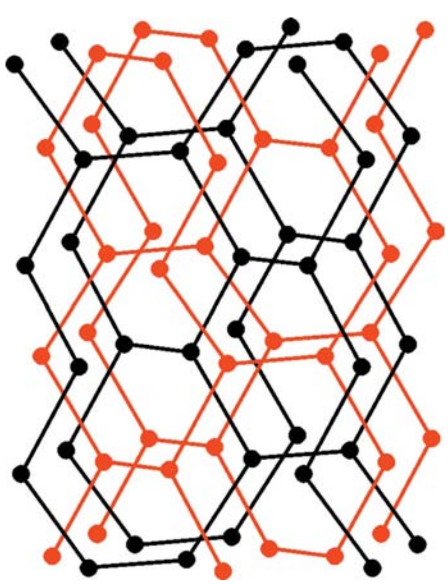

Figure 1
Interpenetrating sphere packings of type $o[3/10/o1]^2$ (*Ccce* 16*i*).

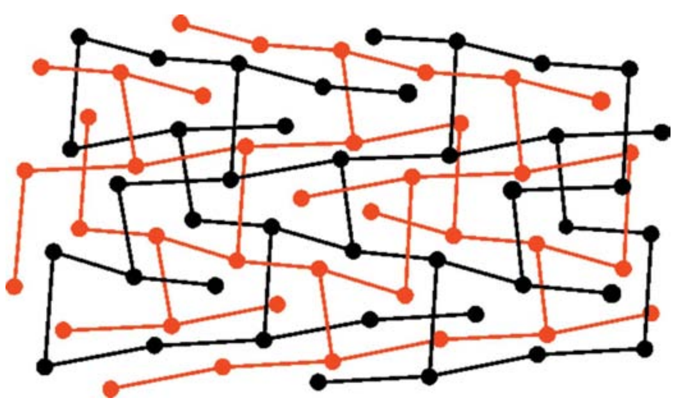

Figure 2
Interpenetrating sphere packings of type $o[3/10/t4]^2$ (*Fddd* 32*h*).

Table 1
Examples for the three new orthorhombic types of interpenetrating sphere packings.

df = degrees of freedom; ρ = density; x, y, z = positional parameters; a, b, c = lattice parameters; d = shortest distance between centres of spheres belonging to different individual packings.

Type	Space group	Subgroup	df	ρ	x, y, z	a, b, c	d
$o[3/10/o1]^2$	*Ccce*	*Pnna* (**b**, **a**, −**c**)	3	0.49967	0.14451, 0.12, 0.17195	2.33806, 3.34566, 2.14339	1.04947
$o[3/10/t4]^2$	*Fddd*	*Fdd*2 (**c**, **a**, **b**)	4	0.67754	0.1, 0.13628, 0.36071	2.21609, 3.30759, 3.37374	1.00395
$o[3/4/t1]^3$	*Fddd*	*Fddd* (3**a**, **b**, **c**)	3	0.34665	0.01975, 0.19462, 0.32675	1.86158, 4.64911, 5.58474	1.12862

three times the value of the minimal density for one individual packing.

Type $t[3/4/t1]^3$ as well as type $o[3/4/t1]^3$ may be derived from the tetragonal type of interpenetrating sphere packings $t[4/3/c6]^3$, which also shows inherent symmetry $I4_1/amd$ 16h. In the general position of *Fddd*, type $t[4/3/c6]^3$ has a two-dimensional parameter region forming the common border between the parameter ranges of $t[3/4/t1]^3$ and $o[3/4/t1]^3$. An individual packing of type 4/3/c6 (Fischer, 1973, 2004) may be visualized as tetrahedra of spheres the centres of which form a tetragonally or orthorhombically deformed diamond configuration. Removing one contact per sphere within such a tetrahedron results in a corrugated quadrilateral of spheres and in a sphere packing of type 3/4/t1, independent of which of the three contacts is omitted. There are, however, two different possibilities for the orientation of such a sphere packing with respect to the triplicate lattice vector and, therefore, two different types of interpenetrating sphere packings are formed.

Table 1 gives parameter values for one example each of the new types of interpenetrating sphere packing normalized to a shortest distance of 1 between sphere centres of an individual packing.

I would like to thank Professor E. Koch for many helpful discussions.

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