

## Three-dimensional model of quasicrystalline atomic structure

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(Received 10 May 1996)

A three-dimensional model of quasicrystalline atomic structure is proposed. The model originates from a 33-atom dodecahedral cluster and involves a strategy allowing us to progressively increase the size of the system using only three basic clusters as building blocks. The structure obtained is characterized simultaneously by dense local atomic packing and by global quasicrystalline properties (intrinsic icosahedral symmetry, the absence of translational order, and self-similarity at different length scales). A 439-atom computer model has been built following the proposed strategy and has demonstrated the possibility to combine global quasicrystalline symmetry with a reasonable local packing of atoms. In order to elucidate the hierarchical nature of the long-range order in the proposed model, it is also analyzed using the disclination network approach. [S0163-1829(96)03042-1]

### I. INTRODUCTION

Modern analytical theories of the atomic structure of quasicrystalline materials involve two principal approaches. The most widespread one makes use of a two-step construction scheme, where (i) a certain “ideal” quasicrystalline lattice is built, using, e.g., three-dimensional (3D) Penrose tiling<sup>1</sup> or a projection of a 6D cubic lattice onto physical 3D space,<sup>2,3</sup> and (ii) this lattice is further decorated with atoms or atomic clusters in that or another way.<sup>4-7</sup> The underlying icosahedral local symmetry of the tiling allows such models to provide a good description of corresponding x-ray diffraction patterns. However, these models are not very helpful for understanding the atomic structure of quasicrystals. First of all, when a quasicrystalline cluster is nucleated and grows from the melt, the attachment and detachment of atoms at the cluster surface are governed by the local environment and local energy gain, and not by the complicated global rules of Penrose rhombohedron packing. Second, even assuming that one can somehow *a priori* identify the tiling, there is no unique recipe of rhombohedra decoration, since the only restriction imposed on a decoration scheme is that of providing a reasonably dense local atomic packing. As a result, the modern decoration models rely very much on the ingenuity of the authors and on analogies to crystalline Frank-Kasper phases<sup>4</sup> or intermetallic compounds with composition close to that of corresponding quasicrystals.<sup>8</sup> Third, the oblate rhombohedra in Penrose tiling are met only as parts of larger aggregates of rhombic dodecahedra, rhombic icosahedra, and triacontahedra.<sup>9</sup> Therefore the models based on Penrose tiling use in fact four basic structural units and the decoration of the larger units cannot be unambiguously defined by specifying the decorations of basic rhombohedra.<sup>10</sup> Moreover, contrary to widespread opinion, there seems to be no reason for the decorations of individual rhombohedra and their typical quasicrystalline aggregates to be unique over the whole quasicrystalline structure.

Another approach attempts to simulate the structure of quasicrystals, following the natural process of quasicrystal growth from an initial nucleation site. This is done either analytically, by defining some “basic” atomic clusters and

then arranging them in space,<sup>11-16</sup> or by molecular dynamics (MD) cooling down of a “melt.”<sup>17,18</sup> The advantage of the MD approach is the immediate determination of the relevant atomic positions without any additional assumptions on the geometric laws governing atomic packing. However, the structures obtained by MD simulations are too complicated to be analyzed without an appropriate reference frame, which can be obtained only from analytical models. Unfortunately, the space packing with the basic clusters used in the existing models cannot be achieved without cluster interpenetration or a noticeable interstitial space between the clusters.<sup>19</sup> Moreover, the lack of an appropriate long-range construction strategy usually does not allow one to indicate a clear way to expand such models to large length scales.

This paper reports a choice of basic atomic clusters and a strategy of quasicrystal expansion using these clusters as building blocks. In Sec. II this strategy is described in terms of a formal iterative process, allowing us to expand the structure from an initial 33-atom cluster up to macroscopic sizes. The strategy involves no interpenetration of basic clusters, whereas the interstitial space is eliminated by a small (“elastic”) distortion of building blocks during the expansion procedure. The resulting structure satisfies both the local requirements of dense atomic packing and the global restrictions imposed by the quasiperiodicity (long-range icosahedral orientational order, self-similarity at different length scales, etc.). In order to demonstrate the nature of the atomic structure far from the nucleation site, a computer model of a 439-atom cluster built following our strategy is described in Sec. III. An efficient visualization of the underlying hierarchical symmetry in the structure proposed is given in Sec. IV in terms of the disclination network approach.

### II. CONSTRUCTION SCHEME

As indicated by MD simulations of the quick cooling down of a binary atomic melt,<sup>18</sup> a liquid metallic alloy can freeze into a metglass, quasicrystal, or Frank-Kasper-type crystal depending on the cooling rate: The lower the cooling rate, the higher the symmetry in the structure obtained. In

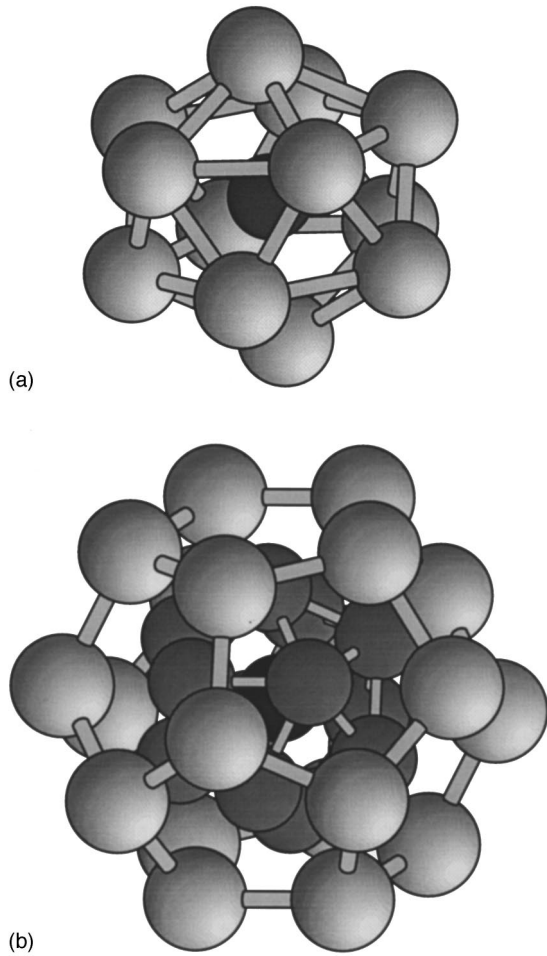


FIG. 1. (a) 13-atomic icosahedral cluster. (b) 33-atomic basic unit  $D_{12}^{(1)}$ .

other words, one can expect that quasicrystals occupy, in a sense, an intermediate position between metglass and icosahedral crystal. Since the same local structure (dominance of the icosahedral local atomic arrangement) is inherent in both metglass and icosahedral crystalline phases, one can expect it to be appropriate for quasicrystals as well. Therefore, the difference between these materials should be manifested in the long-range ordering. Metallic glasses are known to have no long-range order, whereas crystals have full (i.e., both orientational and translational) long-range order. According to general considerations of quasiperiodicity,<sup>1</sup> we assume in our model that only orientational long-range order is conserved in quasicrystals.

Let us start the construction by choosing one atom as a central one and arranging atoms around it in a shell-over-shell way. The icosahedral first coordination shell provides the most energetically favorable local packing of equal-sized atoms.<sup>20,21</sup> Consequently the atoms with icosahedral environment [to be referred to below as Z12 atoms; see Fig. 1(a)] dominate in metglass and Frank-Kasper phases.<sup>22–24</sup> Having in mind the similarity of local ordering in these structures to that of quasicrystals, as well as the expected icosahedral global symmetry, we assume the central atom to be of Z12 type.<sup>25</sup> Already the second coordination shell allows two alternatives: One can place atoms over the centers of either the

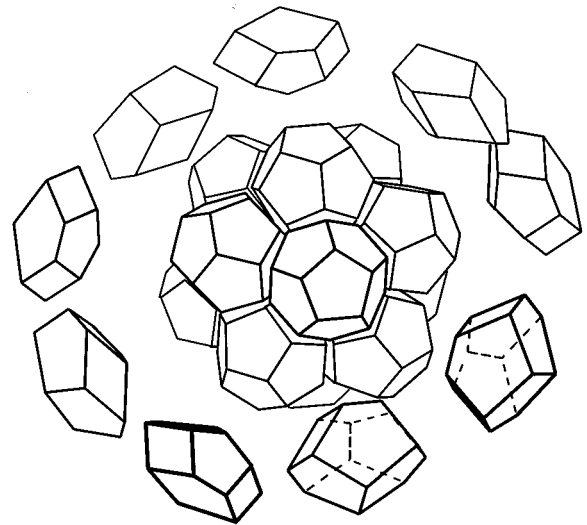


FIG. 2. Schematic representation of the expansion procedure for the dodecahedral units. The invisible edges of two polyhedra in the low right corner are shown by dashed lines.

icosahedron faces or edges. Being supplemented with 12 icosahedrally arranged atoms in the third shell, these alternatives give rise to two basic clusters encountered in the modern models of quasicrystalline structure (see, e.g., Refs. 5, 13 and 14), that is, a 45-atom tricontahedron and a 55-atom Mackey icosahedron, respectively. In the case when the components of a quasicrystalline alloy have approximately the same atomic radii, the tricontahedron cluster provides substantially denser local atomic packing. Therefore we assume that the second shell atoms decorate the faces of the first shell icosahedron, forming a 33-atom dodecahedral cluster  $D_{12}^{(1)}$ ; see Fig. 1(b). This dodecahedral cluster is chosen as a basic unit for our construction strategy, whereas the construction procedure itself is prompted by the following considerations.

Let us represent 13 internal atoms in the basic unit  $D_{12}^{(1)}$  with their Voronoi polyhedra. Since the central atom and the atoms in the first coordination shell are icosahedrally coordinated, their Voronoi polyhedra are slightly distorted dodecahedra put together in a fashion, shown in Fig. 2. The parts of the space left for the vertex atoms of  $D_{12}^{(1)}$  can be easily recognized as quarters of the polyhedron shown in Fig. 3. This polyhedron is nothing but the Voronoi polyhedron for an atom with the coordination number (i.e., number of atoms in the first coordination shell)  $Z = 16$ , introduced by Frank and Kasper<sup>22</sup> as one of the atoms providing locally dense atomic packing and denoted as Z16. The first shell configuration of Z16 is shown in Fig. 4(a).

The Frank-Kasper atoms are known to be typical for icosahedral metglass and crystalline alloys and it seems highly attractive to transform the vertex atoms of  $D_{12}^{(1)}$  into Z16 by adding to our dodecahedral unit cell another 12 such units in a fashion shown in Fig. 2, slightly (“elastically”) distorting these cells so that their surfaces are brought into contact, and then “gluing” these contacting surfaces in such a way that the coinciding atoms at the “glued together” surfaces are united and shared by neighboring units. In order to fill the hollow places in the corners of the construction

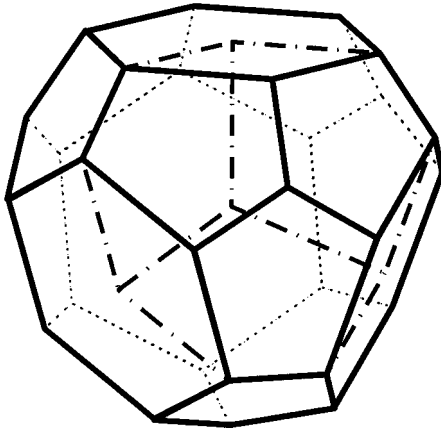


FIG. 3. A Voronoi polyhedron for Z16. The separation into quarters is indicated by dot-dashed lines.

obtained, let us introduce one more basic unit  $D_{16}^{(1)}$  by adding 28 atoms above the faces of the 16-coordinated first neighbor shell of Z16. The resulting second shell, shown in Fig. 4(b), is a scaled copy of the Voronoi polyhedron of the central

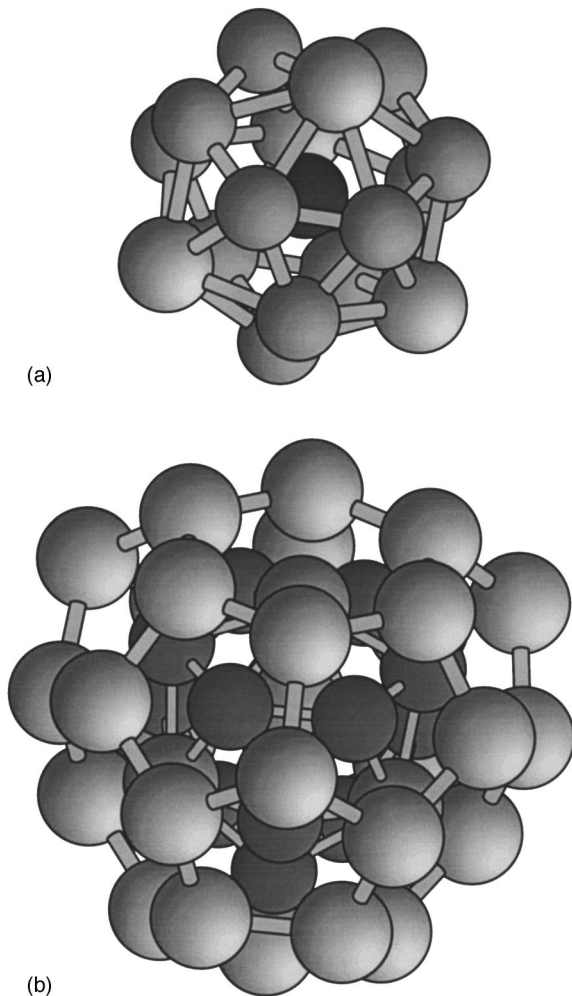


FIG. 4. (a) The first coordination shell of a Frank-Kasper atom Z16. The atoms with six surface neighbors are depicted by larger spheres. (b) 45-atomic basic unit  $D_{16}^{(1)}$ .

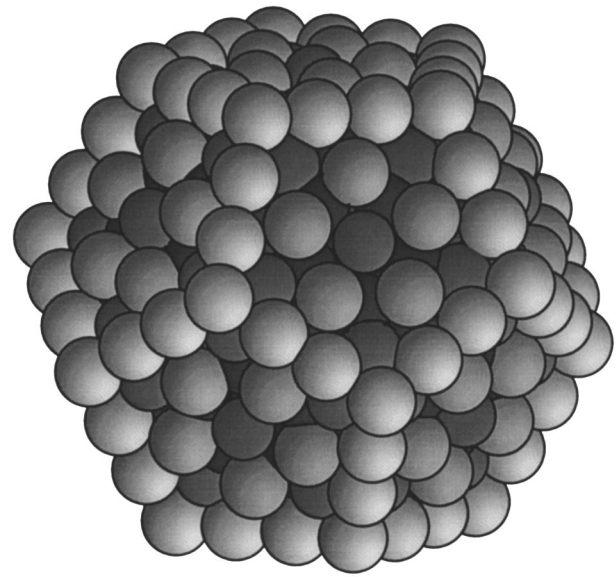


FIG. 5. 439-atomic cluster  $D_{12}^{(2)}$  (the darkness of spheres decreases with increasing shell number).

atom. Note that four atoms in the first shell [depicted in Fig. 4(a) with somewhat larger spheres], are connected to the central atom Z16 by the bonds surrounded by six neighboring atoms. The mutual disposition of these four bonds is tetragonally symmetric in space and thus the  $D_{16}^{(1)}$  unit can be subdivided into four identical quarters, each confined within a body angle made by a trio of neighboring six-coordinated bonds. In order to terminate the expansion step, let us take 20 such quarters and (after appropriate elastic deformation) “glue” their external surfaces to the corresponding surfaces in the hollow corners, as indicated in Fig. 2. The resulting 439-atom arrangement  $D_{12}^{(2)}$  is shown in Fig. 5 and has the same dodecahedral shape as  $D_{12}^{(1)}$ .

Starting from this point, the iterative expansion procedure is straightforward. At the second step we put together 13 second-level dodecahedra  $D_{12}^{(2)}$  and add to the corners 20 quarters of the  $D_{16}^{(2)}$  cluster, which can be obtained from  $D_{16}^{(1)}$  by the expansion procedure similar to that described above, with the only modification that the third basic unit  $D_{14}^{(1)}$  is to be introduced. This basic unit can be constructed in the same way as the other two, i.e., by surrounding a “regular” Frank-Kasper atom Z14 (i.e., an atom with the coordination number  $Z=14$ ) with two coordination shells, as shown in Fig. 6. Such an inflation procedure can be repeated again and again, giving progressively larger sizes of the atomic clusters and involving only inflation of three basic units  $D_{12}$ ,  $D_{14}$ , and  $D_{16}$ . The general inflation rules for basic units at a level  $i \geq 1$  can be schematically described as

$$D_{12}^{(i+1)} = 13D_{12}^{(i)} + 20 \times \frac{1}{4}D_{16}^{(i)}, \quad (1)$$

$$D_{14}^{(i+1)} = 12D_{12}^{(i)} + 3D_{14}^{(i)} + 24 \times \frac{1}{4}D_{16}^{(i)}, \quad (2)$$

$$D_{16}^{(i+1)} = 12D_{12}^{(i)} + 4D_{14}^{(i)} + (1 + 28 \times \frac{1}{4})D_{16}^{(i)}, \quad (3)$$

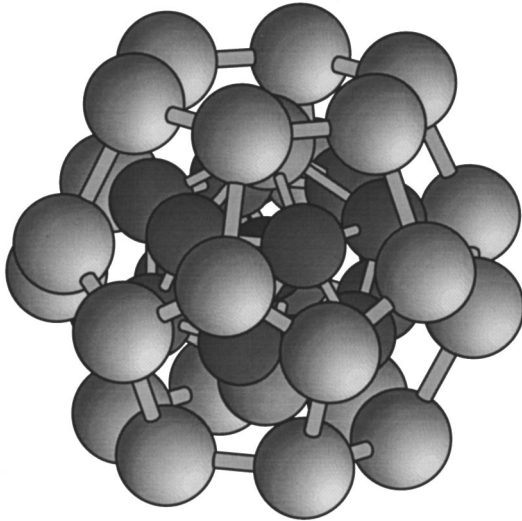


FIG. 6. 39-atomic basic unit  $D_{14}^{(1)}$ .

where the fraction  $1/4$  indicates that only a quarter of the corresponding  $D_{16}$  unit is required to fill in a hollow corner of the corresponding  $(i+1)$ -level unit.

The construction scheme presented indicates that the inflation factors  $f^{(i)}$ , defined as

$$f^{(i)} = d^{(i+1)}/d^{(i)}, \quad (4)$$

where  $d^{(i)}$  is the edge length of the  $i$ th-level polyhedron  $D_{12}^{(i)}$  should be approximately equal to 3.

### III. SIMULATION

At least two points should be addressed in order to justify the relevance of the procedure described above for real quasicrystalline materials. First of all, our construction scheme provides a ‘‘global’’ spatial arrangement of various basic cells, being in this respect similar to Penrose tiling (although the basic structural units are quite different). In contrast to other global schemes, we meet no ambiguities with cell decoration, since the basic units are composed of densely packed atomic clusters and are put together so that only the canonical Frank-Kasper environments<sup>22</sup> with coordinations 12, 14, and 16 are created for interfacial atoms. However, our model involves elastic distortions of basic units and thus can be invalid if these distortions will be too large. The importance of the distortions can be estimated provided we can calculate a radial distribution function for the atoms in the arrangement.

Another specific feature of our model is the presence of a center of symmetry, which implies that quasicrystal growth occurs in a shell-by-shell fashion. This peculiarity does not contradict the experimental observation that quasicrystalline grains usually originate from nucleation sites.<sup>26</sup> Moreover, small (up to 100 nm in diameter) icosahedral quasicrystalline precipitates keep a well-defined dodecahedral shape,<sup>27</sup> just as one would expect from our construction scheme. However, in order for the shell-by-shell growth mode to result in the proposed global structure, the atomic structure of each shell should provide just appropriate accommodation for the atoms of the subsequent shell.

TABLE I. Parameters of the computer model of  $D_{12}^{(2)}$ . The shell radii are in the units of the LJ length parameter  $\sigma$ .

Shell number	Shell type	Atoms per shell	Atom type	Shell radius
S1	I	12	Z12	1.01
S2	D	20	Z16	1.80
S3	I	12	Z12	2.00
S4	TI	60	Z12	2.64
S5	D	20	Z16	2.98
S6	I	12	Z12	2.99
S7	ID	30	Z16	3.56
S8	TT5	60	Z12	3.53
S9	I	12	Z12	4.05
S10	TT3	60	Z12 <sup>a</sup>	4.07
S11	TI	60	Z16 <sup>a</sup>	4.29
S12	TD	60	Z14 <sup>a</sup>	4.63
S13	D	20	Z16 <sup>a</sup>	4.92

<sup>a</sup>Assuming further cluster growth according to the scheme proposed.

Both these considerations have prompted us to apply the construction strategy described above in order to build a model of a 439-atom cluster  $D_{12}^{(2)}$ . First of all, a ball-and-stick model was built shell by shell from plasticine balls (‘‘atoms’’) connected with sticks (‘‘bonds’’) so that both stick ends were kept inside the balls. The ball diameter was equal to  $\sim 0.4$  of the stick length. The parameters of the ball-and-stick model were then used as the input data for a computer program, allowing it to relax the cluster by adjusting the shell diameters and the edge lengths of the rings formed by truncation of regular shell-forming polyhedra, without distorting the original shell symmetry. The relaxation resulted in a noticeable narrowing of the interatomic distance dispersion, even though the surface effects are quite pronounced (e.g., the atoms in the S9 shell are shifted noticeably closer to the  $D_{12}^{(2)}$  surface as compared to the ball-and-stick model).

It was found that the atomic positions in each new shell are unequivocally determined by the structure of the preceding shell, provided we assume that the added atoms are of the Frank-Kasper type. The second-level dodecahedral cluster  $D_{12}^{(2)}$  consists of 13 shells around a central Z12 atom. These shells can be classified into seven types, namely, icosahedron (I), dodecahedron (D), icosidodecahedron (i.e., 30-atom decoration of icosahedron midedges, ID), truncated icosahedron (TI), truncated dodecahedron (TD), and triacontahedron truncated over fivefold (TT5) or threefold (TT3) vertices. Only Z12 and Z16 atom types are met inside  $D_{12}^{(2)}$ . The vertex atoms of  $D_{12}^{(2)}$  should be of Z16 type and those on  $D_{12}^{(2)}$  edges of Z14 type, provided further cluster growth follows the construction scheme proposed. The shell parameters (shell types, number and types of atoms in the shells), as well as the shell radii obtained after the cluster relaxation using monatomic Lennard-Jones potential with the LJ length parameter  $\sigma=1$  are summarized in Table I. Note that the first three shells constitute a 45-atom triacontahedral cluster, Fig. 7, whereas six first shells form a cluster, Fig. 8, used in Ref. 6 for decoration of a ‘‘canonical-cell’’ tiling

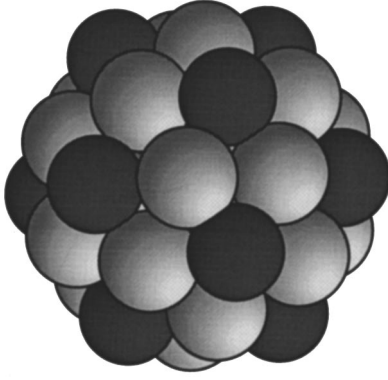


FIG. 7. 45-atomic triacontahedron. Light spheres correspond to shell  $S_2$ , dark spheres to shell  $S_3$ .

(CCT). Similar to CCT, the latter clusters are readily met in our model; however, their relative positioning (along the fivefold symmetry axes) is different from that proposed in Ref. 6.

The distribution of interatomic distances within the relaxed cluster is shown in Fig. 9. The first maximum of the distribution function is well pronounced and has the width of approximately 20% of the average interatomic distance. An average interatomic spacing in the neighboring Z16-Z16 and Z16-Z12 pairs tends to be  $\sim 10\%$  larger than that in Z12-Z12 pairs, indicating the preference for at least two component composition of quasicrystals, with somewhat larger atoms being located in Z16 (and possibly Z14) positions. A similar trend has indeed been observed during the MD quasicrystal formation in a binary system with slightly different atomic radii.<sup>18</sup>

The scaling factor  $f^{(1)}$  in the ball-and-stick model is equal to 2.65, which is very close to the value of 2.618, corresponding to the center-symmetrical Penrose tiling<sup>10</sup> decorated according to Ref. 4. After relaxation  $f^{(1)}$  has increased up to 2.73, however, this value is influenced by surface

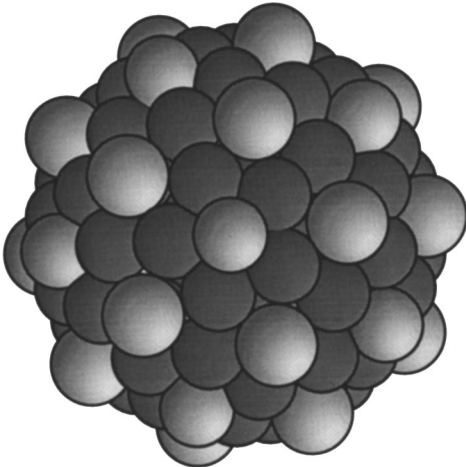


FIG. 8. 137-atomic cluster formed by atoms in the first six shells. Dark spheres, shell  $S_4$ ; larger light spheres, shell  $S_5$ ; smaller light spheres, shell  $S_6$ .

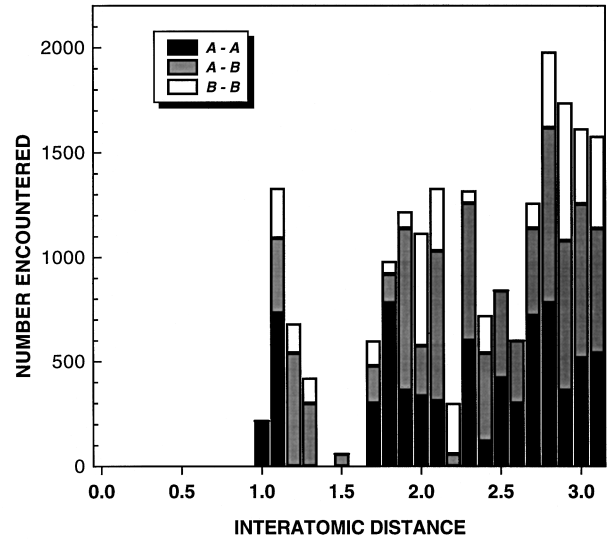


FIG. 9. The distribution of interatomic distances within the  $D_{12}^{(2)}$  cluster relaxed with the LJ potential. Each histogram column is presented as a stack of contributions from atom pairs  $A-A$ ,  $A-B$ , and  $B-B$ , where  $B$  atoms are those located on disclinations and  $A$  inside the matrix. The distances are in the units of the LJ length parameter  $\sigma$ .

effects arising during the cluster equilibration and should not be regarded as a better estimate.

#### IV. DISCLINATION NETWORK APPROACH

A useful alternative to the shell-by-shell description of the structure obtained can be given in terms of the “disclination network” approach, introduced originally by Frank and Kasper (under the name of “basic skeleton”) when considering local atomic arrangements in crystalline alloys<sup>22,23</sup> and further extended to metallic glasses by Nelson.<sup>24</sup> This approach is based on the consideration of interatomic bonds, rather than the atomic positions. Each bond is characterized by the so-called bond coordination number, i.e., the number of the nearest-neighbor atoms forming a ring around the bond. In materials with the dominance of icosahedral local symmetry of atomic environments (including metglasses, quasicrystals, and Frank-Kasper crystals) the majority of bonds have coordination numbers equal to 5, whereas the remaining (“incorrect”) bonds have coordinations equal to 6 or 4.<sup>22</sup> The restrictions of locally dense atomic packing<sup>22,28</sup> do not allow such incorrect bonds to be isolated, but force them to form a closed network. Moreover, all atomic positions in a densely packed arrangement of atoms can be indicated, provided the spatial configuration of the network is determined. In other words, atomic structures with icosahedral local order can be conveniently described in terms of spatial structure of their network of incorrect bonds. It can also be justified<sup>24</sup> that the linear sections of the network (aligned bond chains) can be interpreted in terms of wedge disclinations (in the usual elasticity theory sense<sup>29</sup>).

The introduction of disclination networks in icosahedrally ordered media is to a certain extent similar to the introduction of dislocations in ordinary crystals. However, in contrast to dislocations, the disclinations are not “defects” in the usual sense, but rather an intrinsic structural feature of

icosahedrally ordered media.<sup>31</sup> Moreover, the typical length of straight pieces of these “disclinations” constitutes only several (very often, e.g., in the Frank-Kasper alloys, only one) interatomic distances. Hence, one should not be too straightforward in treating the “disclination network” in macroscopic applications along the same lines, as the dislocation one. Being treated in terms of the disclination network concept, metglass, quasicrystals, and Frank-Kasper crystals differ only in the spatial ordering of the network. In metglass the network is practically disordered,<sup>24</sup> and in Frank-Kasper phases it forms crystalline long-range structures,<sup>23</sup> whereas in quasicrystals one can expect a hierarchical type of disclination ordering.<sup>30</sup>

Our inflation scheme implies that bonds connecting the second-shell atoms in all three basic units  $D_{12}^{(1)}$ ,  $D_{14}^{(1)}$ , and  $D_{16}^{(1)}$  are six coordinated and can be treated in terms of the disclination approach as pieces of the “negative 72° wedge disclinations.”<sup>24</sup> Having in mind that the positions of Z12 atoms in each basic cell are uniquely defined by the cell itself and can be put out of consideration, we may trace only the inflation of the disclination network. At the first step of construction one obtains a (first-level) disclination dodecahedron formed by edges of  $D_{12}^{(1)}$ . At the second inflation step one puts together 13 disclination cells, forming nearly tetragonal disclination nodes, and supplements them with a (second level) dodecahedron of disclinations connecting the vertices of  $D_{12}^{(2)}$  (these second-level disclinations originate in our scheme from the filling of  $D_{12}^{(2)}$  corners with quarters of a unit, originating from a Z16 atom). The subsequent inflation steps lead to the introduction of higher-level disclination networks, each subsequent network being an exact copy of the preceding one, but scaled by an inflation factor. The disclination networks of different levels do not intersect, making a disclination hierarchy. Disclinations of each level play at the same time the role of “superdisclinations” with respect to the disclinations of the preceding level (in the sense that the higher-level disclinations are surrounded by sixfold rings of the lower-level disclinations). The inflation scheme implies that both the atomic and the disclination structures obtained are characterized by intrinsic icosahedral symmetry, the absence of translational order, and self-similarity at different length scales.

Thus the geometry of the disclination network (and the long-range atomic order) in our model is quite different from that in both Frank-Kasper phases and in quasicrystalline decorations derived on their basis.<sup>4</sup> In fact, the hierarchical disclination structure obtained is very similar to that predicted in Ref. 30 as a result of decurving the so-called {3,3,5} polytope, i.e., the regular tetrahedral tessellation of a 3D sphere in a four-dimensional space. This equivalence allows us to obtain one more estimate of the inflation factor. Indeed, when only “negative” disclinations are involved in the decurving of the “ideal” tessellation from a higher-dimensional space (which is the case in Ref. 30), the disclination density in the resulting infinite cluster in the usual Euclidean space tends to a unique nonzero limiting value  $\rho_\infty$ , independent of the decurving procedure details.<sup>24,31</sup> Therefore with the increase of the cluster size the following equation should hold:

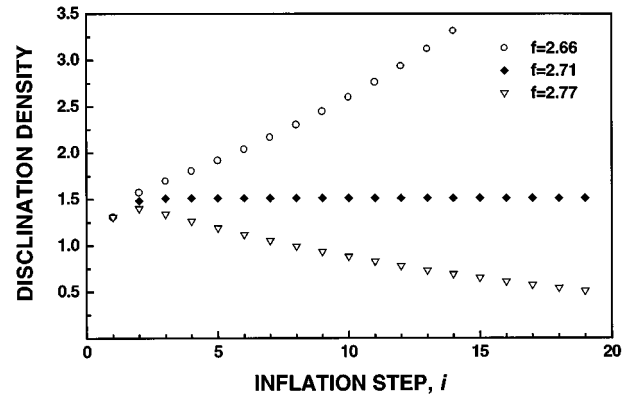


FIG. 10. Disclination density  $\rho^{(i)} \times (d^{(1)})^2$  vs the inflation step number  $i$  at different values of  $f$ .

$$\lim_{i \rightarrow \infty} \rho^{(i)} = \rho_\infty, \quad (5)$$

where  $\rho^{(i)}$  is the disclination density in the cluster after the  $i$ th inflation step.

The full disclination lengths in the  $i$ th-level clusters,  $L^{(i)}$ , are given by

$$L_{12}^{(i)} = 13L_{12}^{(i-1)} + 5L_{16}^{(i-1)} + 10d^{(i)}, \quad (6)$$

$$L_{14}^{(i)} = 12L_{12}^{(i-1)} + 3L_{14}^{(i-1)} + 6L_{16}^{(i-1)} + 12d^{(i)}, \quad (7)$$

$$L_{16}^{(i)} = 12L_{12}^{(i-1)} + 4L_{14}^{(i-1)} + 8L_{16}^{(i-1)} + 14d^{(i)}, \quad (8)$$

where the edge length of the  $i$ th-level polyhedron,  $d^{(i)}$ , is assumed to be the same for all basic units of the same level and we have taken into account that each edge is shared by three polyhedra of the same level. Let us additionally neglect the dependence of the scaling factor  $f^{(i)}$  on  $i$ , i.e.,  $f^{(i)} = f$ . Then

$$\rho^{(i)} = \frac{L_{12}^{(i)}}{f^{3(i-1)} V^{(1)}}, \quad (9)$$

where  $V^{(1)} = (15 + 7\sqrt{5})(d^{(1)})^3/4$  is the volume of the first-level dodecahedron.

The fulfillment Eq. (5) turns out to be very sensitive to the choice of the inflation factor value (see Fig. 10), allowing us to obtain a numerical estimate of  $f \approx 2.714$ . At this value of  $f$  the disclination density converges quickly to a constant value of  $\rho_\infty \approx 1.5(d^{(1)})^{-2}$ . Comparing this value to that obtained in Ref. 31 in terms of the lattice spacing  $a$  of the “ideal” icosahedral tessellation in a curved space, one gets

$$d^{(1)} \approx 1.1a.$$

If we assume that  $a$  represents an interatomic distance between icosahedrally packed atoms within the first-level basic units, this relation clearly indicates an advantage of positioning somewhat larger atoms to the sites laying on disclinations (i.e., those with coordinations  $Z = 16$  and  $14$ ).

At this junction it seems interesting to mention that in quasicrystals of Al-Mg-Cu type the atomic size of one element is indeed approximately 10% larger than the sizes of the other two. The relative numbers of Z12, Z14, and Z16

atoms in the clusters  $D_{12}^{(i)}$ , calculated according to Eqs. (1)–(3), reach their limiting values of 63.2 : 7.0 : 29.8 already at the inflation level  $i=4$  (corresponding to a cluster size of approximately 20–30 nm). Assuming that the larger atoms occupy positions in Z16 and possibly Z14 sites on the disclination network, their concentration should constitute approximately 30–40%, in excellent agreement with experimental values.

## V. CONCLUSIONS

The paper presents a strategy of the quasicrystalline lattice construction, which combines the advantages of an atomistic approach with the well-established global properties (intrinsic icosahedral symmetry, the absence of translational order, and self-similarity at different length scales) required from a quasicrystalline structure. The strategy uses three simple basic atomic clusters as building blocks, which are added together with small elastic distortions, but without intersections or interpenetrations. The structure obtained consists of only canonical Frank-Kasper atoms Z12, Z14, and Z16, thus providing dense local atomic packing in the system.

A 439-atom computer model of a  $D_{12}^{(2)}$  cluster, built according to this strategy, demonstrates the possibility to build

rather large clusters satisfying the composition rules described in the paper.

The interpretation in terms of the disclination network approach reveals the hierarchical nature of the long-range order in the structure obtained, just as one should expect from general considerations.<sup>30</sup>

Both the atomistic modeling and the disclination interpretation indicate the enhancement of the structure stability if the sites at disclinations are filled by somewhat larger atoms than those in the matrix. The filling of disclination sites with somewhat larger atoms requires the concentration of these atoms at a level of 30–40%, which agrees well with the experimental values for quasicrystals of Al-Mg-Cu type.

Finally it should be mentioned that the model presented here can be generalized in order to construct different types of quasicrystalline structures with nonicosahedral global symmetry, starting, e.g., from  $D_{14}^{(1)}$  or  $D_{16}^{(1)}$ . However, this problem will be treated in more detail elsewhere.

## ACKNOWLEDGMENT

The research described in this paper was made possible in part by Grant No. 31300 from the International Science Foundation.

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