

Energetics of clusters with a face-centered-cubic structure

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(Submitted 18 January 1995)

Zh. Éksp. Teor. Fiz. **107**, 2080–2091 (June 1995)

A method for finding the binding energy of atoms in clusters with a face-centered-cubic structure and a pairwise interaction between the atoms at zero temperature is developed. The growth sequence of clusters with a short-range interaction between the atoms, which corresponds to inert-gas clusters, is devised. It is shown that the clusters grow by adding blocks, each of which is an element of a flat surface. Other structures of clusters with a short-range interaction between the atoms are compared. © 1995 American Institute of Physics.

1. INTRODUCTION

Clusters with a pairwise interaction between the atoms at low temperatures can have a face-centered-cubic (fcc) structure and a hexagonal crystal lattice, as well as an icosahedral structure. In each of these structures each interior atom has 12 nearest neighbors, but in the first two structures (close-packed structures) the distances between the nearest neighbors are strictly fixed and equal to the equilibrium distance R_e between the atoms in a diatomic molecule, while in the icosahedral structure these distances differ somewhat from R_e .

When we select the optimal structure of a cluster, the optimal configuration of the atoms in a cluster with a given structure must be determined, and then the binding energies of the atoms in clusters with different structures having the optimal distribution of the atoms for that structure must be compared. This paper is devoted to finding the optimal configurations of the atoms in clusters of fcc structure with a pairwise interaction between the atoms. We start out from inert-gas cluster, i.e., the clusters considered can be cut out from a crystal of an inert gas with an fcc lattice. Then, by moving the surface atoms from certain sites to others, we can determine the optimal configuration of the atoms in a cluster containing an assigned number of atoms. Of course, the optimal arrangement of the atoms in a cluster depends on the interaction potential $U(r)$ of two cluster atoms (r is the distance between the atoms).

The total binding energy E of the atoms in a cluster is expressed in terms of the pairwise interaction potential of the atoms

$$E = - \sum'_{i,j} U(r_{ij}), \quad (1)$$

where r_{ij} is the distance between the i th and j th atoms and the prime indicates that in this sum i is not equal to j and that each pair of atoms is taken into account in the sum only once. Being a convenient model potential, the Lennard–Jones potential often serves as the pairwise interaction potential of atoms (see, for example, Refs. 1–7). Another convenient model pairwise interaction potential is the short-range potential.^{8,9} In a system of bonded atoms the short-range potential acts only between nearest neighbors, while the Lennard–Jones potential also acts between distant atoms.

In order to choose between these two types of interaction potentials, let us compare them by analyzing the parameters of crystals of inert gases.

The sublimation energy of crystals of inert gases per atom in units of the dissociation energy of a diatomic molecule is equal to 6 (half of the number of bonds for each atom) in the case of the short-range interaction potential and to 8.61 (Ref. 10) in the case of the Lennard–Jones potential. The mean value of this parameter for crystals of inert gases is equal to 6.4 ± 0.7 (Refs. 8 and 9), i.e., the short-range interaction potential describes this parameter of crystals of inert gases more accurately. This also applies to the distance between nearest neighbors, which is equal to 1 (in units of the bond length in the diatomic molecule) for the short-range interaction between the atoms, 0.97 (Ref. 10) for the Lennard–Jones potential, and 1.00 ± 0.01 (Refs. 9 and 11) for real crystals of inert gases (with the exception of helium, which is not considered here because of the quantum nature of the system of bound atoms). Another argument in favor of the short-range interaction potential of atoms is that a crystal with the Lennard–Jones interaction potential has a hexagonal crystal lattice,^{12,13} while all inert gases have an fcc crystal lattice.¹⁴ The short-range potential is equally applicable to both structures. In addition, the melting point of a crystal with the Lennard–Jones interaction potential¹⁵ is higher than that of crystals of inert gases and corresponds to their boiling point.

It follows from these facts that the short-range interaction potential more accurately describes the crystal of an inert gas than does the Lennard–Jones interaction potential. Therefore, we shall examine crystals with the short-range interaction potential acting between the atoms. Our goal is to calculate the binding energy of the atoms in such clusters at zero temperature, as well as to compare the values of this parameter for an fcc cluster and clusters with other structures.

2. ENERGETICS OF fcc CLUSTERS

We take the dissociation energy of an unexcited diatomic molecule composed of the atoms under consideration as the unit of energy and the equilibrium distance between the atoms in that molecule as the unit of length. Since there is no long-range interaction in a cluster, the distances between the

nearest neighbors are strictly equal to unity, and the total binding energy of the atoms E is equal to the number of bonds between nearest neighbors. This circumstance greatly simplifies the treatment. In particular, introducing the surface energy of a cluster as

$$E_{\text{sur}} = 6n - E, \quad (2)$$

we obtain the following expression for this quantity:

$$E_{\text{sur}} = \sum_k (6 - n_k / 2), \quad (3)$$

where n_k is the number of nearest neighbors around the k th atom, and the summation is performed over all the atoms. For a very large cluster ($n \gg 1$), the surface energy of the cluster is proportional to the area of its surface $n^{2/3}$. For this reason it is convenient to introduce the specific surface energy of a cluster as

$$A(n) = E_{\text{sur}} / n^{2/3} = 6n^{1/3} - E / n^{2/3}. \quad (4)$$

In the limit of large n this quantity tends to certain constants, which correspond to clusters of definite form. In the general case the function $A(n)$ has a nonmonotonic dependence on n , and the minima of this function [or the maxima of the total binding energy of the atoms in the cluster $E(n)$] correspond to the so-called magic numbers of atoms in a cluster. The magic numbers usually correspond to filled layers, shells, or blocks in the structure of a cluster. Magic numbers ensure the highest stability of a cluster.

Let us now move on to a cluster with an fcc structure and the short-range interaction potential acting between the atoms. One special feature of an fcc structure is that the atoms in this structure can be located in the (100), (110), and (111) planes in the notation usually used,¹⁶ where a plane is characterized by the coordinates of the vector which is perpendicular to it and passes through the origin of coordinates. Since there are six (100) planes, twelve (110) planes, and eight (111) planes, figures of fcc structure containing flat faces, which can number up to 26, can be constructed. If we cut out such clusters from a crystal lattice, we obtain clusters with magic numbers. This approach is the basis for identifying the optimal configurations of the atoms in a cluster and the magic numbers for clusters with an fcc structure.

A more general approach employing this conception was presented in Ref. 17, where it was shown that the magic numbers can correspond to the filling of any of the flat faces of an fcc cluster. There are still the questions of which shapes are magic and which planes must be filled to obtain the magic numbers of atoms in the cluster. These points can be elucidated by comparing the binding energies of the atoms for different figures of the cluster and thereby determining the optimal configurations of the atoms in the cluster. In this paper the problem is solved for clusters with the short-range interaction between the atoms, which simulates inert-gas clusters.

Considering the fcc crystal lattice, we note that it has the O_h symmetry of a cube¹⁸ relative to its center, which corresponds to the following transformations:

$$x \leftrightarrow -x, \quad y \leftrightarrow -y, \quad z \leftrightarrow -z, \quad x \leftrightarrow y \leftrightarrow z. \quad (5)$$

Here it is convenient to select the directions of the axes of the unit cell of the crystal lattice, which has the form of a face-centered cube, as the x , y , and z axes and to select either one of the lattice atoms or the center of the unit cell as the origin of coordinates. In both cases the infinite fcc crystal lattice is maintained under the transformations (5).

We cut out an fcc cluster from the crystal lattice around one of the sites indicated. We call a set of atoms which change places with one another under the transformations (5) a shell of the cluster. The maximum number of atoms in one shell is 48. We introduce the new unit of length $R_e / \sqrt{2}$. In these units an atom with the coordinates x , y , z has 12 nearest neighbors with the coordinates

$$x \pm 1, y \pm 1, z; \quad x, y \pm 1, z \pm 1; \quad x \pm 1, y, z \pm 1. \quad (6)$$

This, of course, applies to the short-range interaction between the atoms, for which the distance between the nearest neighbors depends both on the cluster size and their positions within the cluster. On this basis we can devise a method for determining the optimum configuration of the atoms in an fcc cluster by using the cluster symmetry (5). This symmetry allows us to restrict ourselves to considering only one atom from each shell. Hence, by transposing the surface atoms from some shells to others, we can find the optimal configuration of the atoms for any number of atoms in the cluster. This also makes it possible to obtain the optimum type of growth of the cluster.

This method was previously developed¹⁹ for fcc clusters whose symmetry center corresponds to one of the atoms in the original crystal lattice. Such clusters will henceforth be called clusters with a central atom, and the filling sequence of the shells in these clusters is presented in Table I. However, the center of the unit cell of the fcc crystal lattice can be chosen as the origin of coordinates, and the filling sequence of the shells in such clusters, which we shall call clusters without a central atom, is given in Table II. From these two symmetries, the symmetry which corresponds to the maximum binding energy of the atoms in the cluster must be chosen for every given number of atoms in the cluster. As the cluster grows there is alternation of the optimal symmetry of the fcc clusters, so that in some ranges of cluster sizes the structure with a central atom is optimal, while the structure without a central atom is optimal for others (see Fig. 1).

It follows from an analysis of the data in Tables I and II that a cluster is enlarged by adding to it individual blocks, which include several shells. These blocks are flat elements, which cover the flat faces of the cluster in accordance with the general scheme for assembling clusters.¹⁷ Tables I and II give the optimum configurations of the atoms in each cluster, which have the form of shapes with filled flat faces. The planes to which the filled elements of each cluster belong are indicated.

A comparison of the data in Tables I and II makes it possible to understand the possibilities of the method for finding the optimal configurations of the atoms in a cluster of an assigned size. As an example, we consider a cluster containing 116 atoms. Such a cluster without a central atom corresponds to the filled shape of a truncated octahedron and contains filled 122, 113, and 123 surface shells. Its surface

TABLE I. Growth of clusters with an fcc structure and a central atom.

Filled shells*	n	E_{sur}	Filled block
011(1 - 5)	2 - 13	6 - 42	-
002(4)	13 - 19	42 - 54	-
112(3 - 5) + 022(5)	19 - 55	54 - 114	110
013(4 - 6)	55 - 79	114 - 138	100
222(3) + 123(4 - 6)	79 - 135	138 - 210	111
033(5) + 004(4) + 114(5) + 024(6)	135 - 201	210 - 258	100
233(3 - 5) + 224(5) + 134(5 - 6)	201 - 297	258 - 354	111
015(4 - 6) + 125(5 - 6)	297 - 369	354 - 402	100
044(5) + 035(6)	369 - 405	402 - 414	110
006(4) + 116(5) + 026(6)	405 - 459	414 - 450	100
334(3 - 5) + 244(5) + 235(5 - 6) + +145(5 - 6) + 226(5) + 136(6)	459 - 675	450 - 594	111
055(5) + 046(6)	675 - 711	594 - 606	110
017(4 - 6) + 127(5 - 6) + 037(6)	711 - 807	606 - 654	100
008(4) + 118(5) + 028(6)	807 - 861	654 - 690	100
444(3) + 345(4 - 6) + 255(5) + +336(5) + 246(6) + +156(5 - 6) + 237(5 - 6) + 147(6)	861 - 1157	690 - 858	111
066(5) + 057(6) + 228(5) + +138(6) + 048(6)	1157 - 1289	858 - 894	110
019(4 - 6) + 129(5 - 6) + 039(6)	1289 - 1385	894 - 942	100
455(3 - 5) + 446(5) + 356(5 - 6) + +347(5 - 6) + 266(5) + 257(6) + +338(5) + 248(6) + 158(6) + 167(5 - 6) + 239(5 - 6) + 149(6)	1385 - 1865	942 - 1158	111
077(5) + 068(6) + 059(6)	1865 - 1925	1158 - 1170	110
0010(4) + 1110(5) + 1210(6) + +2210(5) + 1310(6) + 0410(6)	1925 - 2099	1170 - 1230	100
0111(4 - 6) + 1211(5 - 6) + +0311(6)	2099 - 2195	1230 - 1278	100
0012(4) + 1112(5) + 0212(6)	2195 - 2249	1278 - 1314	100

Note. The values in parentheses indicate the number of nearest neighbors.

energy is equal to 180. If a cluster with a central atom of such size is constructed (see Table I), it should contain a spherically symmetric core of 79 atoms and should include blocks of 7 atoms from the 222 and 123 shells. To correct this scheme, three atoms from the 033 shell should be added to two such blocks. The addition of a large block of 17 atoms increases the surface energy of the cluster by 21. To construct a cluster containing 116 atoms, three more atoms (one from the 222 shell and two from the 123 shell) should be added to the core in addition to this block. The surface energy of this cluster with a central atom equals 186, i.e., the structure of the cluster without a central atom is more favorable for a cluster of this size.

Let us construct the optimal structure of the cluster in the coordinate system corresponding to the cluster with a central atom. The optimal configuration of the atoms in the cluster corresponds to a spherical core containing 55 atoms. In addition, it contains 20 atoms from the 013 shell, 24 atoms from the 113 shell, four atoms from the 222 shell, four atoms from the 033 shell, one atom from the 004 shell, four atoms from the 114 shell, and 4 atoms from the 024 shell. Such a cluster is highly asymmetric in this coordinate system and

therefore does not conform to the system of clusters with a central atom, which consists of clusters which are more or less spherically symmetric relative to their center.

This example makes it possible to comprehend the possibilities of the scheme under consideration. By adhering to a definite scheme of symmetric clusters, we can rule out clusters which are highly asymmetric relative to their center. This method thereby ignores extensive rearrangements of the atoms. Therefore, the final result is that the optimal configurations of the atoms are grouped around two structures with a spherical core: a cluster with a central atom and a cluster without a central atom. This follows intuitively from the symmetry of an fcc crystal lattice. The correctness of these statements is supported by the fact that all closed cluster structures which have the form of regular geometric shapes can be constructed using these two symmetries.

An analysis of the geometric shapes cut out from an fcc crystal lattice reveals that an atom located in a (111) plane has nine nearest neighbors, an atom in a (100) plane has eight nearest neighbors, and an atom in a (110) plane has seven nearest neighbors. Therefore, the preferred geometric figures of fcc clusters are bounded by faces lying in (111)

TABLE II. Growth of clusters with an fcc structure and no central atom.

Filled shells	n	E_{sur}	Filled block
001	1 - 6	-	-
111(3)	6 - 14	24 - 48	111
012(3 - 6)	14 - 38	48 - 84	110
003(4)	38 - 44	84 - 96	100
122(3 - 5) + 113(5) + 023(5 - 6)	44 - 116	96 - 180	110
014(4 - 6)	116 - 140	180 - 204	100
223(3 - 5) + 133(5) + 124(5 - 6) + 034(5 - 6)	140 - 260	204 - 312	111
005(4) + 115(5) + 025(6)	260 - 314	312 - 348	100
016(4 - 6)	314 - 338	348 - 372	100
333(3) + 234(4 - 6) + 225(5) + 144(5) + 135(6) + 126(5 - 6)	338 - 538	372 - 516	111
045(5 - 6) + 036(6)	538 - 586	516 - 528	110
007(4) + 117(5) + 027(6)	586 - 640	528 - 564	100
018(4 - 6)	640 - 664	564 - 588	100
344(3 - 5) + 335(5) + 245(5 - 6) + 236(5 - 6) + 155(5) + 146(6) + 227(5) + 137(6)	664 - 952	588 - 756	111
056(5 - 6) + 047(6)	952 - 1000	756 - 768	110
128(5 - 6) + 038(6)	1000 - 1072	768 - 792	100
009(4) + 119(5) + 029(6)	1072 - 1126	792 - 828	100
445(3 - 5) + 355(4 - 6) + 346(5 - 6) + 256(5 - 6) + 337(5) + 247(6) + 238(5 - 6) + 166(5) + 157(6) + 148(6)	1126 - 1510	828 - 1020	111
067(5 - 6) + 058(6) + 229(5) + 139(6) + 049(6)	1510 - 1654	1020 - 1056	110
0110(4 - 6) + 1210(5 - 6) + 0310(6)	1654 - 1750	1056 - 1104	100
0011(4) + 1111(5) + 0211(6)	1750 - 1804	1104 - 1140	100

and (100) planes. In fact, all these shapes can be obtained from an octahedron by cutting off regular pyramids from each of its six vertices. Therefore, we first examine the family of octahedral clusters (Fig. 2a). The surface of an octahedron contains eight triangles in (111) planes. We construct a

family of such shapes, selecting the number m as a parameter of the family such that $m + 1$ atoms are found on each edge

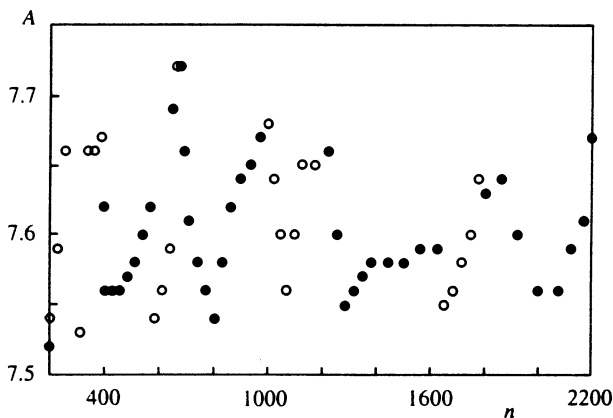


FIG. 1. Specific surface energy of fcc clusters. The filled circles correspond to clusters with a central atom, and the unfilled circles correspond to clusters without a central atom.

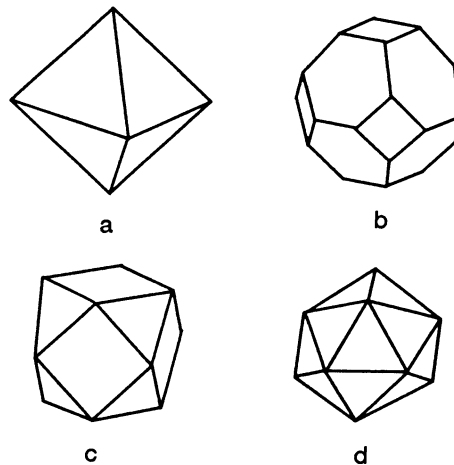


FIG. 2. Geometric shapes which can correspond to the magic numbers of clusters with a pairwise interaction between the atoms: a) octahedron (fcc structure); b) truncated octahedron and tetrakaidecahedron (fcc structure); c) cuboctahedron (fcc structure); d) icosahedral structure.

(the two terminal atoms belong to vertices of the shape). The first shape of the family contains six atoms. The clusters in this family of shapes with even m have a central atom, while octahedral clusters with odd m do not contain a central atom. The number of atoms in the octahedral clusters equals

$$n = 2m^3/3 + 2m^2 + 7m/3 + 1. \quad (7a)$$

To compute the surface energy of each cluster according to Eq. (3), we note that each atom of an edge separating (111) planes has seven nearest neighbors and each vertex atom has four nearest neighbors. In addition, the surface atoms of an octahedral cluster include six vertex atoms, $12(m-1)$ nonvertex atoms located on edges of the octahedron, and $4(m-1)(m-2)$ atoms located within surface triangles. Accordingly, for the surface energy of an octahedral cluster Eq. (3) gives

$$E_{\text{sur}} = 6(m+1)^2. \quad (7b)$$

The truncated octahedrons under consideration have six square (100) faces along with the eight (111) faces. Let us first consider a truncated octahedron (see Fig. 2b), in which there are three atoms on the each side of a square. Such a cluster is obtained from an octahedral cluster by cutting off six pyramids, each of which contains 5 atoms. The number of atoms in this cluster is thus 30 less, and its surface energy is 36 less than that in the octahedral cluster. The surface energy of this cluster can be found by the standard method, since the vertex atoms of the figure each have seven nearest neighbors. We note that the series of magic numbers for fcc clusters listed in Tables I and II (55, 116, 201, 314, 459, 640, 861, 1126, 1804) correspond to this shape.

We move on to a cuboctahedral cluster (see Fig. 2c), which has the form of a truncated octahedral cluster obtained in such a manner that each edge is divided in half when the corresponding pyramid is cut off. Such an operation is possible only for an octahedron with a central atom, i.e., a cuboctahedron is an fcc cluster with a central atom. The surface of a cuboctahedron contains eight triangles with (111) planes and six squares with (100) planes. The cuboctahedron obtained from an octahedron with edges on which there are $2m+1$ atoms has 24 edges, on each of which there are $m+1$ atoms, two of them being vertex atoms. Thus, the surface of a cuboctahedron includes $4(m-1)(m-2)$ atoms within triangles, which have nine nearest neighbors, $6(m-1)^2$ atoms within surface squares, which have eight nearest neighbors, $24(m-1)$ nonvertex edge atoms, each having seven nearest neighbors, and 12 vertex atoms, each having six nearest neighbors. This gives the following expressions⁴ for the number of atoms in a cluster and for the surface energy, which is determined from Eq. (3):

$$n = 10m^3/3 + 5m^2 + 11m/3 + 1; \quad E_{\text{sur}} = 6(2m+1)^2. \quad (8)$$

The first clusters in the family ($n=13, 55$) are magic numbers for fcc clusters.

Let us examine one more figure of a truncated octahedron, viz, a tetrakaidecahedron,⁷ in which each (111) face is a regular hexagon (see Fig. 2b). It can be obtained from an octahedron in which each edge contains $3m+1$ atoms. Then

the length of the edge of each pyramid cut off equals one-third of the length of an edge of the octahedron. We take advantage of the fact that each atom in a (111) plane has nine nearest neighbors, each atom in a (100) plane has eight nearest neighbors, each nonvertex atom on an edge (their total number equals $36m-36$) has seven nearest neighbors, and each of the 24 vertex atoms has six nearest neighbors. Then on the basis of the approach used, we arrive at the following values for the parameters of the cluster under consideration:¹⁹

$$n = 16m^3 + 15m^2 + 6m + 1; \quad E_{\text{sur}} = 96m^2 + 30m + 6. \quad (9)$$

We note that the tetrakaidecahedrons of all sizes considered in Tables I and II ($n=38, 201, 586, 1289$) correspond to magic numbers for an fcc cluster. In addition, we stress the high symmetry of all the figures considered, which is characterized for each of them by three fourth-order symmetry axes and four third-order symmetry axes. It is significant that all the symmetric figures considered can be obtained by the method for assembling fcc clusters considered and belong to one of the cluster structures, i.e., have or do not have a central atom.

3. COMPETITION BETWEEN CLUSTER STRUCTURES WITH THE SHORT-RANGE INTERACTION BETWEEN ATOMS

Along with the fcc structure, clusters with a pairwise interaction between the atoms can have a hexagonal or icosahedral structure, and our problem is to understand which of them is preferable in a given range of cluster sizes. A numerical analysis of the character of the interaction between the atoms in a cluster would probably be most reliable here. Then, after a definite configuration is assigned to the atoms in the cluster, it should be altered so as to increase the binding energy of the atoms (this technique is called cluster relaxation). The optimum distribution of the atoms in a cluster can be determined through cluster relaxation. However, such a procedure is not realistic due to the large number of local maxima of the binding energy, which, for example, amounts to 988 for a cluster consisting of 13 atoms with the Lennard-Jones interaction between the atoms.³ This number increases as the cluster size increases. Therefore, a realistic technique is to "guess" distributions of atoms which are close to optimal and then to relax these distributions (see, for example, Ref. 5). This procedure is simplified in the case of the short-range interaction between the atoms, since the distances between nearest neighbors are rigidly fixed in close-packed structures. Then, we can look through the configurations which claim to be optimal and compare their energies. Essentially this technique was used to compose Tables I and II. In this case the problem is greatly simplified owing to the high symmetry of fcc clusters and the assumption that the optimum distributions of the atoms in a cluster should have a spherical core.

Thus, the general approach to finding the optimum structure of a cluster is to perform an analysis for each of the structures separately and then to compare the binding energies for the optimum configurations of the atoms in each of

these structures. In general this provides an understanding of the role of each particular structure of a cluster with a pairwise interaction between the atoms.

Let us first consider a hexagonal structure. The atoms in fcc and hexagonal structures have identical positions on the (111) plane, while the atoms on the two sides of this plane are arranged differently relative to one another. This common feature of these structures leads to an important phenomenon for metals, which is known as "twinning" and involves the transition from one structure to the other when a (111) plane is intersected.¹⁹ However, this phenomenon is not so significant for clusters with a pairwise interaction between the atoms.

The lower symmetry of the hexagonal structure in comparison with the fcc structure should be noted. This difference is manifested, in particular, by the fact that in symmetric shapes of hexagonal clusters the surface atoms do not form flat faces. Therefore, the surface energy of a hexagonal cluster is generally higher than that for an fcc cluster, and due to the nonmonotonic character of this dependence on the cluster size, hexagonal clusters can have an advantage over fcc clusters at relatively small sizes, at which the icosahedral structure is preferable. Thus, the hexagonal cluster is energetically inferior to the fcc cluster at large sizes and to the icosahedral cluster at small sizes. There are only a few numbers of atoms in the $100 \ll n \ll 1000$ range for which the hexagonal structure is preferable to the fcc and icosahedral structures. Thus, the hexagonal structure is not of great interest for clusters with a pairwise interaction between the atoms.

Let us examine an icosahedral cluster, whose surface consists of 20 regular triangles when the shells are closed (see Fig. 2d). The distances between the nearest neighbors in the same layer differ somewhat (by about 5%) from the distance between nearest neighbors belonging to different layers. However, since these distances are close to the equilibrium distance between the atoms in a diatomic molecule, the total binding energy of the atoms in a cluster is determined primarily by the number of bonds between the nearest neighbors. Since this quantity is greater for clusters with an icosahedral structure than for fcc clusters, the icosahedral structure is preferable for small cluster sizes, and the fcc structure is preferable for larger sizes.

Comparing these structures, we focus on the fact that when the surface layer of an icosahedral cluster is filled, the fcc structure of the surface layer may be more advantageous, since the number of surface-triangle atoms located in the spaces between atoms in the preceding layer is greater for the fcc structure than for the icosahedral structure.^{7,20} Since the interaction between the triangles is stronger for the icosahedral structure, when the upper layer is filled to a significant extent, its fcc structure becomes less favorable than the icosahedral structure. These circumstances were taken into account in constructing the dependence of the total binding energy of the atoms in the fcc and icosahedral clusters on the number of atoms for the short-range interaction between the atoms. This dependence is shown in Fig. 3 for the range of cluster sizes where there is competition between the structures under consideration. The second derivative of the pairwise

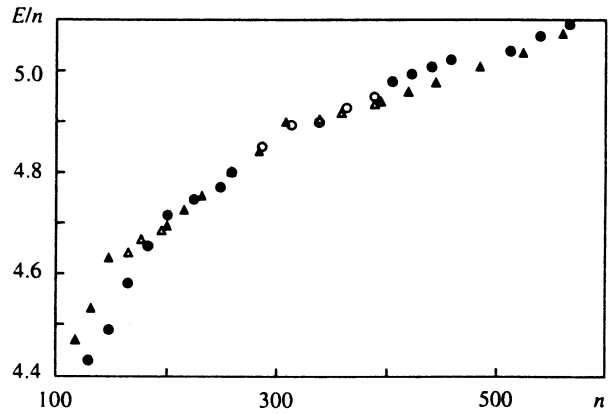


FIG. 3. Specific binding energy of atoms in clusters with short-range interaction between the atoms. The filled circles correspond to fcc clusters with a central atom, the unfilled circles correspond to fcc clusters without a central atom, the filled triangles correspond to clusters with an icosahedral structure for the interior shells and an fcc structure for the surface layer of atoms.

wise interaction potential acting between atoms separated by the equilibrium distance,²¹ which was assumed to correspond to the Lennard-Jones potential [$U''(R_e) = 72$], appears in the results for the icosahedral clusters.

Analyzing the data in Fig. 3, where the binding energies for the magic numbers of atoms in the structures considered were used, we arrive at the conclusion that there is competition between the structures at the numbers of atoms $n = 200 - 500$ in the case of the short-range interaction between the atoms. Then the fcc structure is preferable for some cluster sizes in this range, and the icosahedral structure is preferable for others. In the case of a Lennard-Jones interaction potential acting between the atoms, the competitive region shifts to higher values of n close to 1000 (Ref. 6). We note that the widely used method of comparing given structures on the basis of the Lennard-Jones potential is confined to a comparison of the binding energies in clusters with cuboctahedral and icosahedral structures and filled shells.^{22,23} The convenience of such a comparison stems from the fact that the numbers of atoms in the clusters with filled shells compared coincide. However, such a comparison does not provide a true picture of the competition between the structures, since the cuboctahedral structure is not optimal for fcc clusters.

4. CONCLUSIONS

Thus, the method presented makes it possible to determine the binding energy of atoms in an fcc cluster in a relatively simple manner and the corresponding optimum distribution of the atoms in the cluster for the short-range interaction between the cluster atoms, which correctly describes the interaction in systems of bonded inert-gas atoms. This method can serve as a basis for numerical calculations for a more complicated pairwise interaction potential acting between the atoms.

This research was supported by a grant from the Russian Fund for Fundamental Research.

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Translated by P. Shelnitz