THE TETRAHEDRAL MOTIF IN METAL STRUCTURES

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Abstract

F.C. Frank's demonstration of the stability of the icosahedral configuration to
either of the close-packed ones in thirteen-atom clusters of mutually attracting
hard spheres renewed interest in the occurrence of tetrahedral configurations in
metal alloy structures. This paper reviews some of these developments.

Consider the packing of mutually attracting, by central forces of hard spheres. In two
dimensions the densest, and presumably lowest energy, packing unit is an equilateral triangular
configuration which, when replicated, can fill space to form a hexagonal structure.

In contrast, in three dimensions, the configuration with lowest energy and highest density is a
regular tetrahedron which, by itself, cannot be replicated to fill space and form a close-packed
crystalline structure. The problem then arises of how these tetrahedral configurations,
energetically preferred at short range, are incorporated in, or affect, three-dimensional structures.
In this paper, various ways of including tetrahedral configurations into liquid, glass, and
crystalline structures will be reviewed. Some excellent earlier treatments of this topic are:

M. Hoare [1]
F.C. Frank and J. Kasper [2]
F. Yonazawa [3]
J.F. Sadoc and R. Mosseri [4]
L. Bartell [5]
be formed by one-to-one
configurations. However, if the
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by F.C. Frank’s
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“frustrate” crystallization
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that this preference must
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itetrahedral configurations
metalloid (B) liquid alloys
Rothery and Anderson [8]
s must hold energetic
ordinarily deep eutectic at
ature is roughly 540°C
accord with what the

Hume-Rothery-Anderson model would predict. The melting temperature of the ordered
intermetallic phase with composition Au4Si is only 5°K below that of the actual eutectic.

Deposition from the pure metal vapor or dilute solution onto cold substrates might, initially,
result in the formation of icosahedral, or other polytetrahedral, clusters (these have been labeled
“amorphons”). These amorphons would continue to enlarge, and upon mutual impingement form
a microquasicrystalline or, perhaps, a glassy structure. There is the intriguing possibility that
below a certain thickness a quasicrystalline structure might be preferred, thermodynamically, to a
microcrystalline one at the same atomic density. However, we know of no experimental evidence
of a direct transformation from a micro-crystalline to a quasi-crystalline state.

A considerable number of metal alloys form structures in which icosahedral groups of atoms,
as defined by Dirichlet constructions, are prominent components of the overall structure. Kasper
also noted other coordination polytetrahedra which often appear in these structures. Frank and
Kasper then examined these phases and outlined the general principle for inclusion of tetrahedral
configurations in alloy structures. These alloys have come to be known as “Frank-Kasper
phases”.

Since icosahedral configurations appear to be important components of liquid structure, it
seems that their resistance to nucleation of crystals with major polytetrahedral groups might be
much lower than that to simple close-packed structures. This comparison can be made roughly
in terms of the scaled, with thermodynamic melting temperature, \(T_M\), undercooling at the onset
of measurable crystal nucleation, \((T_M-T_N)/T_M = a\). For most pure metals, \(a\) is of order 0.2 to
0.25. At this time, information on those metals in which polytetrahedral groupings are
prominent in their structures is rather sparse. However, recent studies at the Institut für
Raumsimulation in Cologne by D. Holland-Moritz, D.M. Herlach and their coworkers, have
indicated that \(a\), for phases with major icosahedral or other polytetrahedral configurations in their
structures, do indeed exhibit a values (~0.10) substantially below those with crystalline close-
packed structures. The Cologne results were obtained by observation of droplets which were
levitated electromagnetically. Earlier observations by Bendersky and Ridder [9] on the formation
The melting temperature of the ordered face-centered cubic (FCC) structure occupies a major role in the study of the formation of intermetallic compounds. The research by Hume-Rothery and Anderson [4] and others has provided insights into the formation of these compounds. The interaction between the FCC and tetrahedral (B) liquid alloys is a topic of interest, particularly in the formation of ordered compounds.

The Frank-Kasper structure, which is often observed in ordered alloys, exhibits a preference over simple cubic structures. This preference is due to the reduced energy associated with the formation of these structures. The Hume-Rothery model predicts the formation of these structures in the liquid phase, and the model is supported by experimental observations.

The formation of these structures is not limited to liquid alloys. The precipitation of ordered structures from the FCC matrix is also observed in solid solutions. The precipitation of these structures is a function of the thermal stability and the driving force for the formation of these structures.

The precipitation of these structures is also influenced by the size of the superstructure units. The larger the size of the superstructure units, the more stable the structure. This stabilization is due to the reduced thermal fluctuation and the increased interaction between the superstructure units.

In summary, the formation of the ordered face-centered cubic (FCC) structure in the liquid phase is a complex process that is governed by the interaction between the FCC and tetrahedral (B) liquid alloys. The Frank-Kasper structure is a preferred structure due to its reduced energy, and the formation of these structures is influenced by the size of the superstructure units and the thermal stability of the superstructure units.
of quasicrystals from suspended droplets of Al-Mn alloy indicated in the condensed structure an extremely high concentration (~10^{18}/cm^3) of microquasicrystallites.

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References


**PhysicS AND METALlU**

W.L. Johnson, 138-78 Keck

The basic factors governing the development of complex multico structure is characteristic of conventional cast systems. The key kinetic and these systems are outlined. Fina crystal shape to produce unique properties is described.

**Glass Formation in Met**

The early work of Turk demonstrated that a thermodynamically local fluctuation in the liquid in a nucleation is decisive. In Turnbull:

\[ R = \frac{\text{nucleation rate}}{\text{unit volume}} \]

where \( n \) is the rearrangement decreases with undercooling. In Turnbull:

\[ W \propto (16\pi/3)\gamma^2/\Delta g^2 \]

where \( \Delta g \) is the specific enthalpy of crystallization (both per unit \( n \) as a constant, and \( T_\infty \) the mean approximation).

The rate of atomic rearrangement coefficient in the melt is through the Stokes-Einstein relation that dates the early 20th century, the temperature dependence: