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Characterization of the Locally Ordered Regions in Short-Range Ordered α-Phase Cu–Al Alloys*†

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Abstract

The ordered domain structure present in the α-phase Cu–Al alloys investigated by Epperson, Fürnrohr & Ortiz [*Acta Cryst.* (1978), A**34**, 667–681] is determined by an extension of the computer method developed recently by Epperson [*J. Appl. Cryst.* (1979), **12**, 351–356] for analyzing a Gehlen–Cohen type simulated structure for a binary, f.c.c., locally ordered alloy in terms of nearest-neighbor atomic configurations. The dominant ordered feature of the more concentrated of these alloys is the existence of randomly dispersed Borie–Sparks tetrahedra; that is, four nearest-neighbor Al atoms arranged tetrahedrally about a Cu atom. The majority of these tetrahedra are isolated; however, as many as three or four are occasionally found to be joined in fragments of a Cu_3Au-type antiphase-shift structure. This extended ordered structure also incorporates the Cu_3Au-type ring configuration, another principal characteristic structural feature of these Cu–Al alloys. As a typical example, a Cu–14·76 at.% Al alloy quenched from 923 K and annealed for 1580 h at 423 K was found to contain 87 such locally ordered regions in an 8000-atom model. Of these 'domains', 74 were isolated tetrahedra and the remainder consisted of pairs of tetrahedra joined such that their central atoms were mutual second-nearest neighbors. For this alloy and heat treatment, the locally ordered regions of this type amount to about 14 volume % of the microstructure and contain 32% of the Al in the alloy. The average (spherical) domain size is only 3·4 Å. Not only are the locally ordered regions very small, but there are also perceptible imperfections in the packing sequence.

Introduction

One of the principal goals of diffuse-scattering investigations of concentrated alloys has been that of understanding locally ordered structures in terms of charac-

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teristic local atomic configurations and their more extended correlations, which result in the existence of ordered regions or domains. A straightforward extension of the computer method developed by Epperson (1979) to determine the complete spectrum of nearest-neighbor (n.n.) atomic configurations in locally ordered, binary, f.c.c. alloys permits one to probe the Gehlen–Cohen simulated structure (GC structure) for additional information about the ordered domains in terms of structure, domain size and the size distribution, volume fraction and composition. The purpose of this contribution is to outline briefly how this analysis is effected and to apply it to the determination of the ordered domain structure in the α-phase Cu–Al alloys investigated recently by Epperson, Fürnrohr & Ortiz (1978), henceforth denoted by EFO.

Background

Techniques developed over a period of years now permit a rather sophisticated analysis of local atomic ordering in concentrated, substitutional, binary alloys. Within the kinematic approximation, the coherently scattered diffuse intensity due solely to the distribution of atoms *on* the average lattice sites can be expressed, in Laue monotonic units, as

$$I(h_1,h_2,h_3) = \sum_l \sum_m \sum_n \alpha_{lmn} \cos 2\pi(h_1\,l + h_2\,m + h_3\,n), \quad (1)$$

where l, m and n comprise a triplet of integers which specifies an occupied lattice site in relation to an arbitrary origin, and the h_i are continuous variables in reciprocal space. The Fourier coefficients α_{lmn} are the Cowley–Warren order parameters (Cowley, 1950) defined by

$$\alpha_{lmn} = 1 - P_{lmn}^{A|B}/X_B, \quad (2)$$

where $P_{lmn}^{A|B}$ is the conditional probability of finding a B-type atom at site lmn relative to an A atom at the local origin, and X_B is the atom fraction of species B. Thus, the structural information about the local atomic order is contained in a set of statistical parameters.

Generally, the experimental intensity data are further corrupted by modulations of the Laue monotonic due to the fact that the atoms do not reside precisely at the average lattice sites. These size-effect modulations can, however, be separated by schemes based on the work by Borie (1961) and Borie & Sparks (1971), the currently most advanced separation method being that of Tibbals (1975) and Georgopoulos & Cohen (1977). The size-effect separation effectively reduces the problem to that represented by (1), and it is not necessary to pursue this aspect of the problem further here.

Originally, the method of analyzing the order component of the coherent diffuse scattering data was to assume a model for the local atomic order and to compute and compare the order coefficients with the experimental values. This procedure demanded a great deal of insight, lacked generality and was quite tedious if detailed model calculations were carried out. Gehlen & Cohen (1965) recognized, as had Cowley (1950), that the lower-order α_{lmn} constrain the values that the higher-order parameters can assume and used this fact to justify generating a large computer model which represents the average structure, as described by the experimental α_i. In effect, this computer simulation affords one the possibility of recovering some real-space structural details from the statistical order parameters.

Even though one could now 'see' the atoms, it was still a prohibitive task to extract quantitatively the structural information from this simulation because of the inherent nonrepeating nature of the local atomic order. The scope of this problem and the frustrations encountered in earlier attempts to recognize and quantify the locally ordered regions in the GC structure has been ably described by Gragg, Bardhan & Cohen (1971). Epperson (1979) has recently shown that the complete spectrum of nearest-neighbor atomic configurations can be determined from the GC structure, with no assumptions in addition to those already invoked in its production. This analysis allows a quantitative assessment of the n.n. configurations present in the alloy and how they vary with composition, heat treatment, *etc.*

However, these basic structural units are small by definition; in fact, they are often too small to reveal fully the locally ordered structure. This was recognized by EFO as a limitation of the method, and they pointed out that it would be possible to extend the searching procedure so as to make additional relevant information contained in the GC structure readily available to the investigator.

Method of analysis

In order to perform a detailed structural characterization of an alloy, as depicted by its GC structure, it is convenient to designate the sites in the first coordination shell about a given lattice site as shown in Fig. 1. For a substitutional, f.c.c. binary alloy, there are 4096 possible configurations of the atoms about an arbitrary site; however, the symmetry of the face-centered cubic lattice reduces this number to a more manageable 144 crystallographically distinct n.n. configurations. With a master catalogue of the 4096 possible n.n. configurations, it is a relatively simple task, aided by a modern digital computer, to characterize *each* site in the GC structure, and this tagging and searching procedure is what Epperson (1979) used to determine the complete spectrum of n.n. configurations present in an alloy.

In principle, this same scheme could be used to designate, and to allow one to search out, any proposed atomic configuration (or its structural equivalent) which might be contained in the GC structure. However, this direct method becomes very cumbersome as the number of atoms in the cluster gets larger, due to the sheer number of permutations and the necessity to program individually for each cluster of interest. Fortunately, there is an easier way to accomplish much the same goal.

Since we now have a convenient designation of all possible n.n. configurations, one should be able to use these fundamental structural entities to specify more extended correlations, that is locally ordered regions. One should be able to devise a rather general computer code based on this principle which, to a large extent,
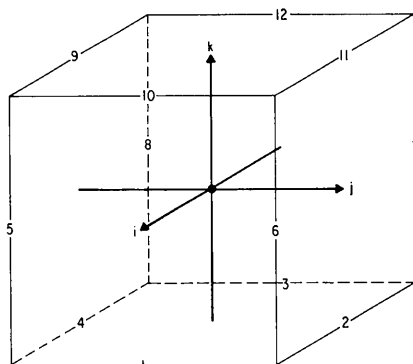

Fig. 1. Site designation used for the nearest-neighbor configurations in f.c.c. systems. For a complete listing of the configurations, see Table 1 in Epperson (1979).
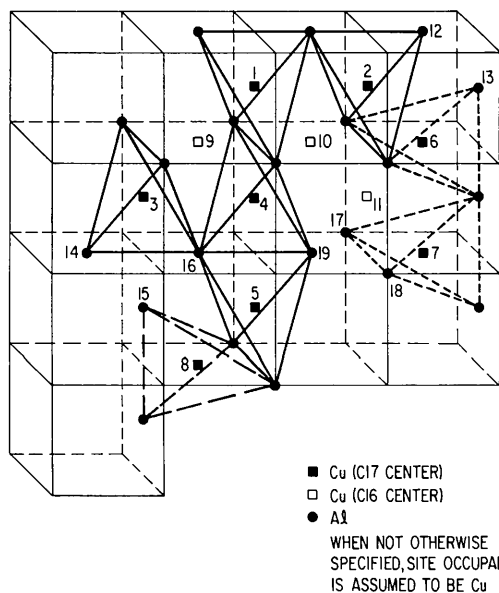

■ Cu (CI7 CENTER)
□ Cu (CI6 CENTER)
● Aℓ
    WHEN NOT OTHERWISE
    SPECIFIED, SITE OCCUPANCY
    IS ASSUMED TO BE Cu

Fig. 2. Segment of an ordered structure illustrating various-sized domains which are composed basically of the Borie–Sparks tetrahedra.

reduces the problem to that of deciding which of the 144 n.n. configurations comprise the ordered region and how they are interconnected. How this works can be illustrated by the extended, irregularly shaped, ordered region shown in Fig. 2. Suppose one wishes to search the GC structure for ordered domains consisting of Borie–Sparks tetrahedra (here denoted as $C17$ units) whose center atoms are mutual second-nearest neighbors. With this specification, the following domains will be indicated: one consisting of the five tetrahedra centered about sites 1, 2, 3, 4 and 5; a second made up of the two $C17$ units about sites 6 and 7; and a third which is only the 'isolated' tetrahedron at site 8. It is arbitrarily assumed that all atoms in the first coordination shell about each of the defining n.n.-configuration central atoms belong to the domain.

One sees that the above specification results in some Cu_3Au-type rings (denoted as $C16$ units) being incorporated in the domain; i.e. at sites 9, 10 and 11. The particular assemblage of clusters illustrated here could not occur in the α-phase Cu–Al alloys due to the strict prohibition against first n.n. Al–Al pairs (see Tables 1 and 2 of EFO). If one relaxes the restriction on connectivity and allows the $C17$ units to be either first- or second-nearest neighbors, all eight of the tetrahedra shown here belong to the same ordered domain. On the other hand, the specification of the $C17$'s which are mutual first-nearest neighbors results in two multiple domains centered on sites 2 and 6 and 5 and 8, all others being considered isolated. Flexibility of this type is desirable in allowing the investigator to probe the GC structure for fragments of various ordered structures and to examine their perfection. The computer code now in use allows one to specify the ordered domains in terms of any one or any combination of the 144 n.n. configurations and to have these specified n.n. units joined as: (1) first n.n., (2) second n.n., or (3) first- or second-nearest neighbors. A listing of the 144 possible n.n. configurations is given in Table 1 of Epperson (1979).

Perhaps a very brief digression would be in order to emphasize that the probing techniques under discussion are not narrowly confined to this Cu–Al alloy system. It is not uncommon in locally ordered systems for nucleation to occur independently throughout a grain, with the resulting microstructure being a mixture of the possible variants, especially in stoichiometric alloys. This represents a special kind of imperfection which too is amenable to the searching scheme outlined above. Consider, as an example, the Ni_4Mo-type structure shown in Fig. 3. In our notation, the ideal long-range ordered structure can be thought of as a single variant composed of the $C8$ n.n. configurations aligned parallel to one of the coordinate axes and with all basic n.n. units having a common sense of rotation. For this structure, there are six possible variants, and the program now in use is equipped with an option so that, if

desired, these six variants can be classified separately. It would be moderately simple to incorporate similar options for details of other structures.

As indicated above, for the present purpose all atoms in the first coordination shell about each central atom in the specification configuration(s) are considered to belong to the ordered region or domain. Based on the foregoing definition of a cluster and its interface, one can easily estimate the volume fraction of ordered domains, their mean composition and the fraction of the minor constituent which is contained in the ordered regions. Also, one obtains the domain size distribution in terms of the number of specified n.n. configurations each extended, ordered cluster contains. These parameters are valid irrespective of the shape of the extended cluster. Even though crude, an estimate of the mean domain size is helpful in characterizing the state of order in an alloy. This estimation is affected by treating the ordered domains, as being spherical, clearly an oversimplification but nonetheless useful if one does not attempt to ignore this assumption.
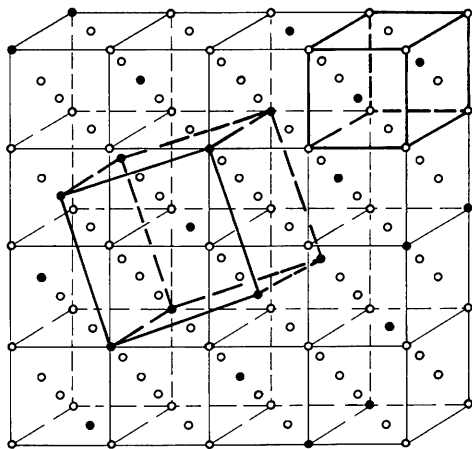

Fig. 3. Schematic illustration of one variant of the Ni₄Mo-type structure.

Results and discussion

The short-range order in α-phase Cu–Al alloys containing 9·13, 13·56 and 14·76 at.% Al has been investigated recently by Epperson, Fürnrohr & Ortiz (1978), primarily using high-angle X-ray diffuse-scattering techniques and single-crystal samples. They determined, without *a priori* assumptions, the complete spectrum of first-nearest-neighbor atomic configurations. Their Cowley–Warren order coefficients are listed in Tables 1 and 2 and the corresponding n.n. configurations of Al about Cu atoms are given in Tables 3 and 4 of EFO. They argued that the main features of the short-range order could best be described in terms of two of the n.n. configurations: $C17$'s consisting of four nearest-neighbor $A1$ atoms arranged tetrahedrally about a Cu atom, as proposed by Borie & Sparks (1964), and $C16$'s consisting of a planar array of four n.n. Al atoms about a Cu atom in the Cu₃Au-type ring configuration. Their (EFO) analysis also revealed a transient increase in the $C9$ population when the Cu–14·76 wt% Al alloy was quenched from 923 K and annealed isothermally at 523 K. For the $C9$ configuration, all the atoms are contained in {111}-type planes. This latter behavior was interpreted as evidence for operation of the Suzuki (1952) mechanism; that is, the very localized interaction of solute Al atoms with stacking faults which, in this case, are produced by slight deformation of the single crystals induced by the quenching operation. In the former case, however, their analysis was recognized as being incomplete, inasmuch as they were unable to specify the extended correlations among the 'highly ordered' $C17$ and $C16$ n.n. configurations. The searching techniques discussed in the previous section now make it possible to address this problem. In the discussion to be presented here, it is implicitly assumed that the 'close fitted' GC structure represents the best estimate of the average short-range ordered structure;

Table 1. *Domain structure summary of* Cu-Al *single crystals annealed for* 1580 h *at* 423 K

These data are derived from the order coefficients measured by Epperson, Fürnrohr & Ortiz (1978).

N.n. configurations comprising the domains (how connected) / Number of such connected n.n. configurations	Cu–13·56 at.% Al			Cu–14·76 at.% Al		
	$C17$ (2nd shell only)	$C17$ (1st or 2nd shell)	$C16$ (1st or 2nd shell)	$C17$ (2nd shell only)	$C17$ (1st or 2nd shell)	$C16$ (1st or 2nd shell)
1	47	45	20	74	59	37
2	5	3	2	13	14	9
3	0	2	0	0	3	4
4	0	0	0	0	1	1
Total number of such ordered domains	52	50	22	87	77	51
Volume fraction of domains (%)	8·7	8·7	3·8	14·4	14·4	10·1
Composition (atom fraction)	0·2968	0·2968	0·3033	0·2951	0·2951	0·2988
Mean (spherical) radius (Å)	3·4	3·4	3·8	3·4	3·5	3·5

hence our effort will be directed toward extracting structural details from this simulation, leaving a discussion of its possible shortcomings for the following section.

For 8000-atom models* corresponding to the three alloy compositions, very few of these ordered n.n. configurations were found in the random alloys:† in the 9·13 at.% alloy, none; in the 13·56 at.% alloy, one $C16$ and two $C17$'s; and in the 14·76 at.% alloy two $C16$'s and five $C17$'s. In each case, none of these ordered n.n. units was within either the first or second coordination shell of another such unit.

In the 9·13 at.% Al alloy annealed for 1580 h at 423 K, significant numbers of $C16$'s and $C17$'s appear, 11 $C16$'s and 10 $C17$'s, which represents 6·0 and 5·5% of the total Al content, respectively. All the tetrahedra were isolated in the sense that no other tetrahedron was found within either the first or second coordination shells. The $C16$'s were likewise isolated. In two instances $C16$'s and $C17$'s were found to be coordinated; however, the extremely low number density makes it difficult to decide if this is evidence for some order extending beyond the first coordination shell. On the other hand, the population of the isolated $C16$'s and $C17$'s is sufficient to indicate that these ordered units indeed represent relatively stable n.n. atomic configurations in this alloy.

When one considers the more concentrated α-phase Cu–Al alloys, there are clearly some extended correlations as shown by the data in Table 1. Firstly, note the distribution of tetrahedra whose centers are mutual second-nearest neighbors. This packing sequence represents 'perfect fragments' of a Cu_3Au-type antiphase shift structure, of the kind sketched in Fig. 4. A natural

consequence of this extended ordered array is the occurrence of the Cu_3Au-type ring configurations as well. For the ideal $M = 1$ antiphase-shift structure, these n.n. configurations occur in the ratio 2 : 1, and this is probably the reason EFO observed $C17$ to $C16$ ratios ranging from 1·5 to 2·2 for a variety of heat treatments of the Cu–14·76 at.% alloy.

Not all the tetrahedra are arranged in this manner, however, as is clearly seen by an examination of the domain size distributions for the different connectivity specifications. That is, some of the Cu-atom tetrahedron centers are mutual first-nearest neighbors. The strict prohibition against Al–Al first-nearest-neighbor pairs means that the only spatial arrangement which accomplishes this requirement is that shown in Fig. 5. Thus, one concludes that, although the most frequent ordered regions are the small fragments of the antiphase-shift type structure, there are also some ordered domains that are best characterized as defect variants.

It should not be assumed that those locally ordered domains are embedded in a perfectly random matrix. This can be seen in Fig. 6, where the composition in the various coordination shells, averaged about all the

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* Since all our models (GC structures) consisted of 8000 atoms, we will henceforth dispense with giving the specific size designations.
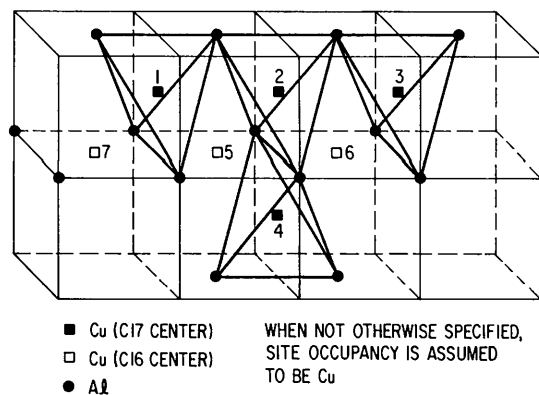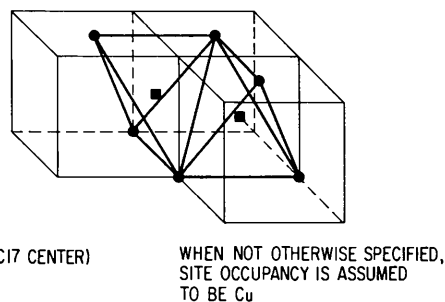
† Computer generated such that $a_i = 0$, $i = 1, 7$.

■ Cu (C17 CENTER)
● Al

WHEN NOT OTHERWISE SPECIFIED, SITE OCCUPANCY IS ASSUMED TO BE Cu

Fig. 5. An illustration of imperfections found in the locally ordered domains of the α-phase Cu–Al alloys.

■ Cu (C17 CENTER)
□ Cu (C16 CENTER)
● Al

WHEN NOT OTHERWISE SPECIFIED, SITE OCCUPANCY IS ASSUMED TO BE Cu

Fig. 4. An example of a 'perfect fragment', although irregular in shape, of the Cu_3Au-type antiphase-shift structure. Notice that both $C16$'s and $C17$'s are incorporated in this structure.
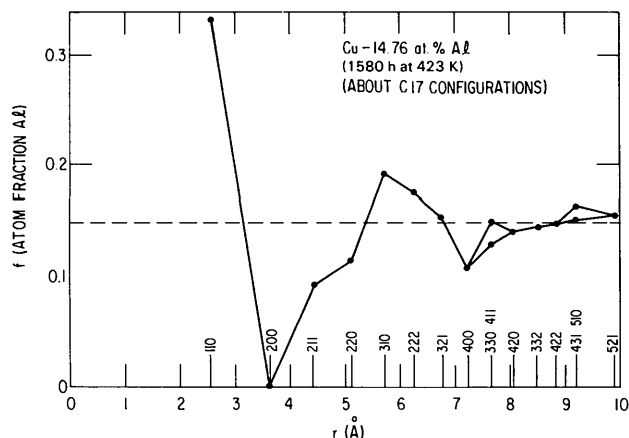

Fig. 6. The composition in the various coordination shells averaged about all the tetrahedra centers in the GC structure for the Cu–14·76 at.% Al alloy annealed for 1580 h at 423 K.

tetrahedra, is plotted. Clearly, the interfaces are somewhat diffuse. According to the data given in Table 1, there are about 7.9×10^{26} m^{-3} locally ordered regions consisting of isolated tetrahedra or tetrahedra connected either as first- or second-nearest neighbors. This translates to a mean interparticle distance of about three unit-cell dimensions. The fact that the composition averaged about the $C17$ units has converged to the mean bulk composition after roughly 2·2 unit-cell dimensions is a clear indication that there is no significant correlation in the positions of the locally ordered regions; that is, they are essentially randomly distributed. As defined in a previous section, about 8·7 and 14·4 volume % of the microstructure is made up of these locally ordered regions, for the Cu–13·56 and 14·76 at.% alloys, respectively. This corresponds, respectively, to 20 and 32% of the Al in the alloys.

The sizes of the locally ordered regions are also worth comment: as shown in Table 1, the mean size (spherical radius) was only about 3·5 Å. The largest of the 'perfect' $C17$ clusters observed was 3·95 Å and contained 22 atoms, seven of which were Al. This accounts for the fact that Epperson, Kostorz, Ortiz, Fürnrohr & Gerstenberg (1979) found no evidence for significant volume segregation when investigating these alloys with small-angle neutron scattering. Weak small-angle scattering was observed, but it could be attributed convincingly to dislocation scattering.

Summary

X-ray diffuse-scattering measurements are currently among the most advanced techniques for obtaining quantitative information about the structure of concentrated, weakly ordered alloy systems. The work reported here, a continuation of that reported earlier by Epperson, Fürnrohr & Ortiz (1978) and Epperson (1979), addresses the problem of characterizing the small locally ordered regions, or ordered domains, present in this alloy system which give rise to well known high-angle diffuse-diffraction effects (Borie & Sparks, 1964).

Recently developed computer techniques make it possible to extract fine details about the extended correlations among the basic structural units, the nearest-neighbor atomic configurations. It is argued that the average locally ordered structure in these α-phase Cu–Al alloys is best described in terms of small regions consisting of $C17$ and $C16$ units; the Borie–Sparks tetrahedra and Cu$_3$Au-type ring configurations, respectively. Most of the tetrahedra are isolated in the sense that no other such units are centered within the first two coordination shells. However, significant numbers of these tetrahedra so coordinated as to result in small randomly dispersed fragments of a Cu$_3$Au-type antiphase-shift structure. This structure also incorporates the Cu$_3$Au-type ring configuration, an ordered n.n. configuration which is also prominent in the simulated structure of these alloys. Furthermore, imperfection within some of the domains can be detected. Rather than having all the $C17$ tetrahedra chained as mutual second-nearest neighbors, occasionally they are mutual first-nearest neighbors. One can visualize these defects as resulting when pairs of linear $C17$ 'domains' intersect at right angles. Why this imperfection results is at present not understood.

These perfectly ordered domains amounted to about 14 volume % of the microstructure in the case of the Cu–14·76 at.% Al alloy. But the locally ordered regions were quite small, only 3·4 to 3·5 Å mean radius. None larger than 3·95 Å were detected.

The analytical methods used here are not restricted to this alloy system. In fact, they would be usable immediately for any f.c.c., substitutional binary alloy, and it would be feasible to construct similar codes at least for the b.c.c. equivalents. It is perhaps worth pointing out that the same procedures would apply to alloy systems in which there is a tendency towards clustering, as opposed to the short-range order investigated here. It would be interesting to investigate the locally ordered structure in a clustering system to see if there is evidence for a depleted shell about the GP zones as proposed, for example, for the Al–Ag system by Walker & Guinier (1953). Because extended clusters containing many more atoms are involved, this would require larger computer models for adequate statistics. Detailed structural information of this type is obviously needed if one is to understand fully such phenomena as diffusion, oxidation resistance, and strength characteristics of alloys.

It must be clearly recognized that the amount and quality of information one can hope to obtain from this type of analysis is limited ultimately by the fidelity of the Gehlen–Cohen structure, assuming the diffraction data are properly corrected for contributions other than that of the distribution of the atoms on the average lattice sites. That is, how closely do the experimental Cowley–Warren order coefficients, which themselves are defined statistically, constrain the structure? Except in the special case of long-range order, the structure simulation does not yield a unique solution (Clapp, 1971). Intuitively, one feels that the fidelity decreases as does the degree of order in the system. This general problem has also been discussed by Gehlen & Cohen (1965), Gragg, Bednarz & Cohen (1970), Gragg, Bardhan & Cohen (1971), Williams (1970, 1978) and Epperson (1979); the last demonstrated that, for a given selected set of order coefficients, the GC structure was reproducible within about 5% in terms of the population density of the various n.n. configurations when the first six α_i are 'close' fitted. The fidelity of the computer simulation with respect to more extended correlations has not been investigated, but one should

be cautious when fine structure is present in the diffuse diffraction pattern. Given the current state of art with respect to extracting information from the simulated structure, additional theoretical guidance about the model fidelity would be highly desirable.

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Termination of Planar Defects in the Amphibole Mineral Nephrite Observed by High-Resolution Electron Microscopy

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Abstract

Termination of planar defects has been observed in the amphibole mineral nephrite [$Ca_2(Mg,Fe)_5(Si_4O_{11})_2(OH)_2$]. Isolated terminations, which disrupt the crystal structure, are rare, but the cooperative termination of two defects, in which the total number of silicate chains is conserved and structural disruption is minimized, is more common. Two different kinds of cooperative termination have been observed. Occasionally, defects are seen to terminate and shift their line of propagation through a crystal.

Introduction

Nephrite is a fine-grained, compact form of actinolite. A recent refinement of the structure of this amphibole was carried out by Mitchell, Bloss & Gibbs (1971) ($C2/m$, $a = 9.89$, $b = 18.20$, $c = 5.30$ Å, $\beta =$

104·64°). In essence, the structure consists of doubly-linked chains of SiO_4 tetrahedra running parallel to [001]: layers of chains are separated by cations in distinct sites, with a large vacant site between those chains disposed back-to-back (Fig. 1).

The presence of planar defects in various amphiboles (Hutchison, Irusteta & Whittaker, 1975; Veblen, Buseck & Burnham, 1977) and nephrite in particular
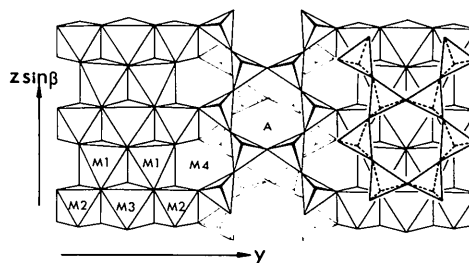

Fig. 1. The $C2/m$ amphibole structure projected along x.