

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 $[\text{Ca}_2(\text{Mg,Fe})_5(\text{Si}_4\text{O}_{11})_2(\text{OH})_2]$. 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

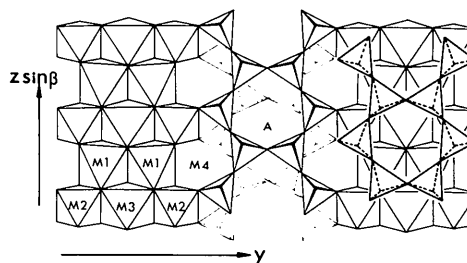


Fig. 1. The $C2/m$ amphibole structure projected along x .
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(Hutchison, Jefferson, Mallinson & Thomas, 1976; Mallinson, Hutchison, Jefferson & Thomas, 1977; Jefferson, Mallinson, Hutchison & Thomas, 1978; Mallinson, Jefferson, Thomas & Hutchison, 1980) has been established by means of high-resolution electron microscopy. Such defects consist of single, triple and higher multiply linked chains of silicate tetrahedra coherently inserted into the double-chain matrix and are a means by which a given crystal can accommodate compositional fluctuation. Computation of image contrast (Mallinson *et al.*, 1980) has shown that, in an image observed under appropriate microscope conditions of a thin crystal tilted with $[100]$ parallel to the beam, white (020) fringes, with separation *ca* 9 Å, correspond in position to the centres of double chains of the crystal structure and that this applies equally to defects as to the regular structure. Thus the absence of a (020) fringe and an increase of $b/4$ in the fringe spacing indicate the incorporation of a single chain, while two adjacent white fringes, separation *ca* 4.5 Å, indicate the position of a triple chain.

Experimental

Nephrite specimens (kindly made available by the British Museum) from the following sources were studied: New Zealand; Monterey County, California; Mashaba Chrome Mine, Victoria, Zimbabwe-Rhodesia; Fraser River, British Columbia; South Sea Islands; Jordansmuhl, Breslau, Silesia. Small pieces were crushed to a fine powder, dispersed in chloroform and deposited on a copper grid coated with a holey-carbon film. The specimens were examined in a Siemens 102 electron microscope operated at 100 kV. Areas of thin crystals projecting over holes were suitable for tilting and subsequent imaging. Except where stated, all crystals were tilted such that $[100]$ was parallel to the beam.

Results and discussion

Single terminations

The lone termination of a fault has rarely been found. Such an occurrence must disrupt the structure where the result is a different number of silicate chains either side of the termination. An example is shown in Fig. 2, where at *A* a triple chain terminates, resulting in a difference of one chain on either side of the boundary *BC*. Faults *D* and *E* are continuous.

Double terminations

A more common occurrence than a single termination is that where two defects are observed to terminate in conjunction. The two terminations ensure

that the total number of chains over a given area is conserved, with minimum disruption to the crystal structure. This has been observed to happen in two different ways.

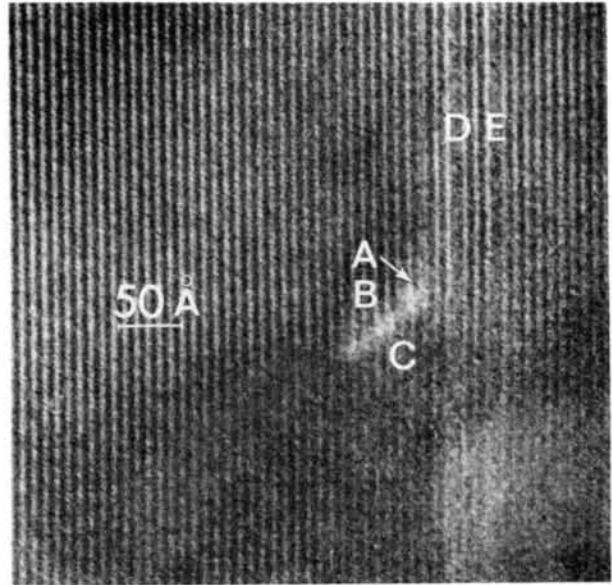


Fig. 2. The termination of a triple chain at *A* disrupts the structure in the region *BC*.

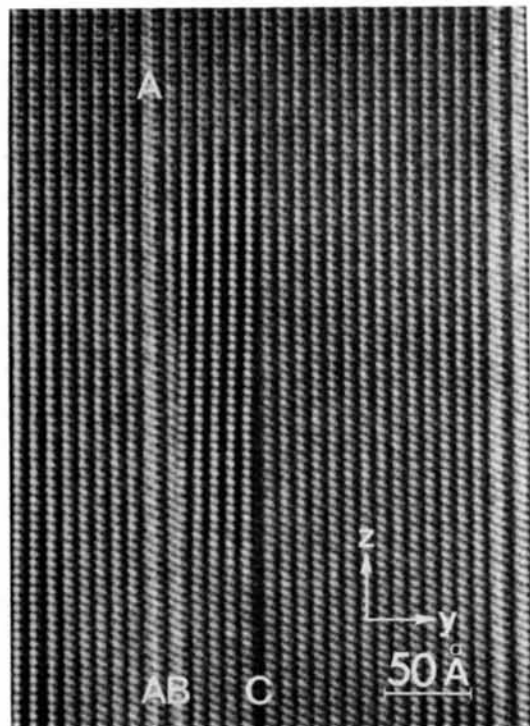


Fig. 3. The associated terminations of triple chain *B* and single chain *C* occur with little structural disruption.

(1) The most common form of double termination is as seen in Fig. 3. Defect *A* is a continuous triple chain. Adjacent to *A*, in the lower half of the micrograph, defect *B* is another triple chain, while, close by, defect *C* is a single chain. Proceeding along [001], both defects *B* and *C* terminate gradually and only defect *A* is present in the top half of the micrograph. As two double chains form from *B*, and *C* is eliminated, the total number of silicate chains remains the same and the structure of only that part of the crystal between the terminations is disturbed, as evinced by the (020) fringe bending towards *B*. Fig. 4 is a possible structural explanation of this phenomenon. The chains are represented by strips, trapezoidal in cross section, reflecting their disposition as tip-to-tip or back-to-back,

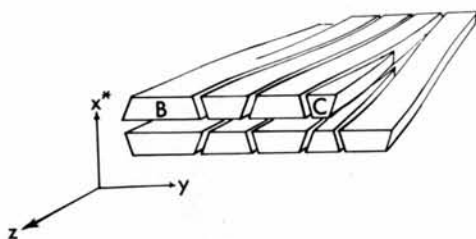


Fig. 4. Possible structural explanation of the terminations shown in Fig. 3.

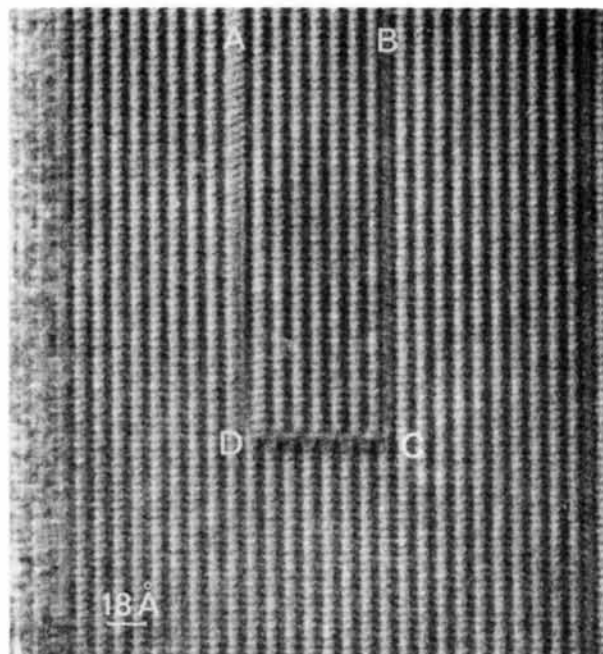


Fig. 5. A less commonly observed type of associated defect termination. Triple chain *A* and single chain *B* terminate with a planar fault joining the two.

with the cationic sites omitted. Since alternate chains along [010] have their tetrahedra in opposing orientations, the elimination of a chain presents structural problems in that no two, unconnected, adjacent chains can have their tetrahedra pointing in the same direction. One possible solution is the incorporation of a type of screw dislocation (Burgers vector $\frac{1}{2}a[100]$) which brings chains of opposing tetrahedral orientations from different levels along [100] together to maintain the regular structure. Such changes are well represented in the image, Fig. 3, where the increase in contrast of those fringes between the two terminations reflects a slight change in orientation of that particular part of the crystal with respect to the beam, caused by the incorporation of the two screw dislocations.

(2) A less commonly observed type of double fault termination can be seen in Fig. 5, taken with [102] parallel to the beam, an orientation which still shows the relative disposition of the silicate chains. Defect *A*, a triple chain and defect *B*, a single chain, apparently terminate at the same position along [001]; the two terminations are separated by a planar fault *CD*, across which the double chains are in misregistry. The total number of silicate chains in the whole region remains the same and there is apparently little disturbance to the crystal structure. Fig. 6 is a possible structural explanation, with the silicate chains projected down x^* . Across *CD* those chains that meet with opposing tetrahedral orientations may join by edge-sharing of tetrahedra. Distortion of tetrahedra in this region is necessary and this is perhaps reflected in the image contrast, which also indicates that the region of distortion is very limited.

Defect changes of position

Terminations which result in defect position shifts, so that the progress of the fault through the crystal is non-linear, have been observed for triple chains (Mallinson *et al.*, 1980) and Fig. 7 shows an example apparently involving single chains. Two single chain defects *A* and *C* shift position to *B* and *D* through

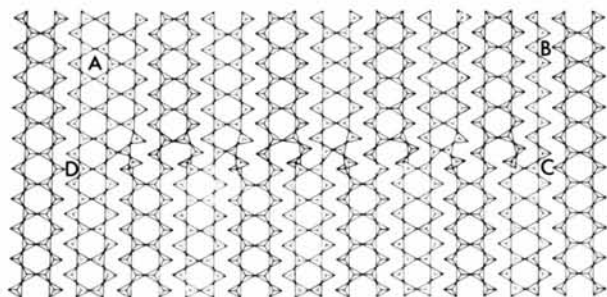


Fig. 6. Possible structure plan of the terminations shown in Fig. 5.

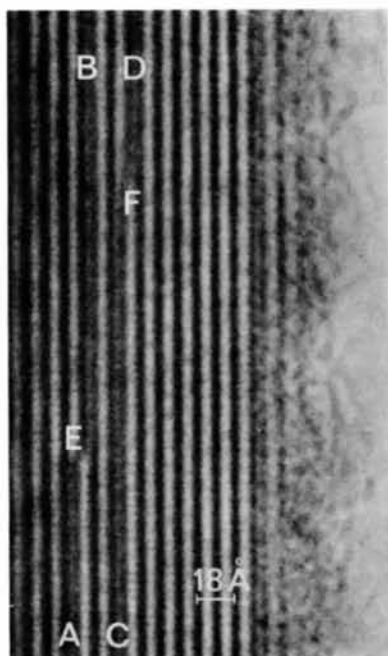


Fig. 7. Micrograph, taken with $[102]$ parallel to the beam, showing single chain defect position shifts, through terminations E and F .

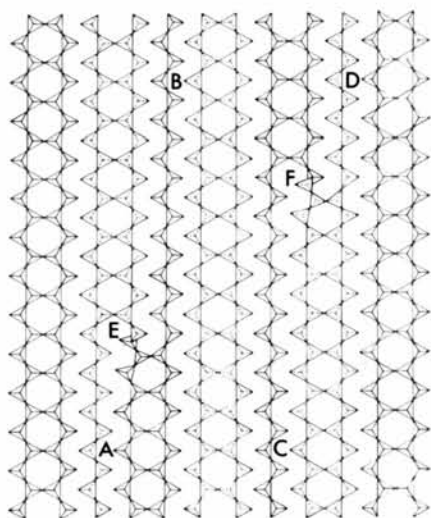


Fig. 8. Possible explanation of the behaviour of the silicate chains as shown in Fig. 7.

terminations E and F . A possible structural explanation is shown in Fig. 8. Again, the edge-sharing of tetrahedra is postulated at the fault terminations in order to minimize disruption to the silicate backbone.

Conclusions

The presence of defect terminations in nephrite is an unusual occurrence, implying that, in the vast majority of cases, chemical composition is constant along $[001]$ in a given crystal. Where compositional changes necessitate defect termination, however, this is nearly always accommodated by the linked termination of two defects in order to conserve the number of silicate chains. In this way, structural disruption is minimized to very small regions, implying that, in nephrite, the integrity of the silicate chain backbone is of paramount importance to the stability of the crystal structure.

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