Dislocations in Energetic Materials. 2. Characterization of the Growth-Induced Dislocation Structure of Pentaerythritol Tetranitrate (PETN)

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Abstract
The predominant dislocation types in crystals of pentaerythritol tetranitrate (PETN) grown from solution have been observed and characterized using transmission X-ray topography. The dislocation characterization, carried out by contrast variations, was aided and simplified by comparison of observed dislocation line directions with those calculated from the theory of preferred line directions of Klapper [Habilitationsschrift (1975). RWTH, Aachen]. With a few exceptions, the dislocations observed were induced during growth. Eight different types were identified comprising all possible Burgers vectors up to and including \langle 111 \rangle. Of these, one was pure edge, the remainder being of mixed character. The relative frequency of occurrence of the dislocation types is discussed, together with factors influencing dislocation contrast and characterization.

1. Introduction
Crystal defects, in particular dislocations, have been observed to play a significant role in such processes as crystal growth (Burton, Cabrera & Frank, 1951; Van Enckevort, 1982; Hooper, Roberts & Sherwood, 1983), solid-state polymerization (Meyer, Lieser & Wegner, 1978), solid-state decomposition (Thomas, 1969; Thomas & Williams, 1971; Herley & Levy, 1972; Begg, Halfpenny, Hooper, Narang, Roberts & Sherwood, 1983), the electrical properties of solids (Begg, Roberts, Sherwood, Groth-Andersen & Jacobsen, 1981; Monkowski, 1981) and the performance of solid-state devices (Meieran, 1980). Speculations have also been made of their involvement in both the slow and rapid decomposition of energetic solids. Singh (1956) has observed the thermal decomposition of mercury fulminate to occur preferentially on (010) and (100) planes. He interpreted this in terms of a redistribution of dislocations on these planes during heating. Similarly, Jach (1962) proposed preferential decomposition at dislocations to account for the observed thermal decomposition kinetics of lead azide. A detailed understanding of the behaviour and properties of dislocations in crystalline explosives are of interest not only to qualify such speculations but also because it has been proposed that the initiation of explosives by impact may occur through the formation of localized 'hot spots' following plastic deformation (Bowden, 1958; Elban & Armstrong, 1981).

The properties of a dislocation are, in general, strongly dependent on its character and on whether or not it is formed during growth or induced mechanically at a later stage in growth. Dislocation characterization is therefore an important step towards understanding defect properties and relating these to the behaviour of the bulk material. X-ray topography (Lang, 1959) provides a useful tool in the analysis of growth-induced dislocation configurations in large nearly perfect single crystals. Using this technique, we have determined the nature of the growth-induced dislocation structure of the important organic secondary explosive pentaerythritol tetranitrate (PETN).

The basic method of characterization of dislocations by X-ray topography uses the invisibility criteria \( g \cdot b = 0 \) and \( g \cdot b \times l = 0 \), where \( g \) is the diffraction vector and \( b \) and \( l \) are the Burgers vector and line vector, respectively, of the dislocation (Lang, 1978). The method is frequently hindered by a number of factors.

1. The criteria apply strictly only to elastically isotropic media.
2. Mixed dislocations seldom become completely invisible. This is particularly significant in the analysis of growth dislocations, which rarely follow low-indexed line directions and are often of mixed character.
3. Dislocations are often decorated by solvent or other impurities. This can modify the strain field of the dislocation thus making it visible in all reflections. This again can be a common occurrence with growth dislocations.
4. The unambiguous Burgers-vector assignment of any dislocation requires invisibility or near invisibility in at least two reflections. Each reflection defines a plane in which the Burgers vector lies and the line of intersection defines \( b \) itself. It is often the case that the
particular reflection or reflections required are unavailable. This may be due to (a) systematic absences; (b) the required reflection may be too weak to give dislocation images suitable for analysis. This is a common problem with organic materials due to the small atomic scattering factors, (c) some reflections will be inaccessible due to the geometry of the slice plane available.

5. Superimposition of defects causes difficulty in establishing whether or not a dislocation has become invisible.

As will be confirmed below several of these factors present problems in attempting a dislocation analysis in the present case. In several publications Klapper has shown that growth-induced dislocations normally follow well-defined directions in crystals. He has developed a theory based on the linear anisotropic elastic properties of a defective lattice which confirms the observed orientations. In this paper we have used theoretical calculations of the preferred line directions in PETN to supplement the extinction contrast data. In this way a satisfactory determination of the character of the growth dislocation structure can be obtained despite the problems noted above.

2. Theoretical analysis of growth-induced dislocation types

A preliminary topographic examination of PETN single crystals (Halfpenny, Roberts & Sherwood, 1984a) has revealed that, almost without exception, the dislocations were straight and followed a number of discrete well defined line directions. Few of these line directions were low indexed. Most dislocations originated from either inclusions or growth-sector boundaries. Such features are characteristic of growth-induced dislocations (Klapper, 1980).

As an aid to the characterization of these dislocations, it is valuable to consider the various growth dislocation families which might be expected to occur in PETN. This involves, firstly, establishing the probable Burgers vectors, \( \mathbf{b} \). The line direction of a given growth dislocation is defined by its Burgers vector and the growth direction, \( \mathbf{n} \), of the growth sector in which it lies. It is, therefore, also necessary to consider the possible combinations of \( \mathbf{b} \) and \( \mathbf{n} \).

2.1. Burgers vectors

PETN crystallizes in the tetragonal space group \( P\overline{4}_2_1c \) with \( a=b=0.938 \) nm and \( c=0.67 \) nm (Booth & Llewellyn, 1947). Since the unit cell is primitive there is no halving of lattice translations due to centring. For energetic reasons, the shorter lattice translations are generally favoured as dislocation Burgers vectors. On this basis, Burgers vectors longer than \( \langle 111 \rangle \), although not completely discounted, were considered improbable. The shortest Burgers vectors for PETN are listed in Table 1.

Table 1. PETN Burgers vectors

| \( \mathbf{b} \) | \( |\mathbf{b}| \) |
|-----------------|-----------------|
| 001             | 0.67            |
| 100             | 0.938           |
| 101             | 1.153           |
| 110             | 1.327           |
| 111             | 1.486           |

2.2. Dislocation families

Crystals of PETN exhibit the forms \{110\} and \{101\} only. Consequently there are twelve growth directions; four corresponding to the \{110\} growth sectors and eight to the \{101\} sectors. Together with the 13 probable Burgers vectors, this gives a total of 156 possible combinations of \( \mathbf{b} \) and \( \mathbf{n} \). In this instance the sense of the Burgers vector is unimportant since it does not influence the calculation of the line direction of the growth dislocation. Hence only 13, rather than the full 26, specific Burgers vectors up to and including \( \langle 111 \rangle \) are considered. Many of the possible combinations of \( \mathbf{b} \) and \( \mathbf{n} \), and therefore the dislocation line directions they define, are symmetrically equivalent. The 156 possible combinations can be reduced to 16 non-equivalent combinations. These are listed in columns 2 and 3 of Table 2.

2.3. Calculations of preferred dislocation line directions

The potential configurations of dislocations in the growing crystal were evaluated using Klapper's (1975) theory. The calculation is based on linear anisotropic elasticity theory with the following basis.

The preferred line direction of a particular dislocation corresponds to that in which the dislocation energy per unit growth length is a minimum, \( \text{i.e.} \)

\[
W = \frac{E}{\cos \alpha}
\]

where \( E \) is the dislocation energy per unit length of straight dislocation and \( \alpha \) is the angle between the line vector \( \mathbf{l} \) and the growth normal \( \mathbf{n} \).

The energy of a linear dislocation consists of two terms, the elastic energy \( E_a \) of the long-range strains surrounding a dislocation and the dislocation core energy \( E_c \). The former is given by

\[
E_a = \frac{K|\mathbf{b}|^2}{4\pi} \ln \frac{R}{r_0},
\]

where \( K \) is an energy factor that depends on \( \mathbf{l}, \mathbf{b} \) and the elastic properties of the crystal. \( R \) and \( r_0 \) are the outer and inner cut-off radii of the dislocation concerned. The core energy of dislocations cannot be calculated with any degree of accuracy. It can be neglected without serious error, however, since it is usually estimated to be at least an order of magnitude smaller than \( E_a \). Hence, the dislocation energy per unit
Table 2. Preferred dislocation line directions in PETN

<table>
<thead>
<tr>
<th>Type</th>
<th>Character</th>
<th>Angle between $b$ and $\mathbf{n}$ (°)</th>
<th>$\varphi$ (°)</th>
<th>$\theta$ (°)</th>
<th>$\Delta W^*$ (eV nm$^{-1}$)</th>
<th>$E$ (eV nm$^{-1}$)</th>
<th>% screw component</th>
</tr>
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<tbody>
<tr>
<td>la</td>
<td>Edge</td>
<td>90</td>
<td>45</td>
<td>90</td>
<td>0.6</td>
<td>19</td>
<td>0</td>
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<tr>
<td>lb</td>
<td>Mixed</td>
<td>90</td>
<td>0</td>
<td>36</td>
<td>0.3</td>
<td>46</td>
<td>0</td>
</tr>
<tr>
<td>2a</td>
<td>Mixed</td>
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<td>67</td>
<td>90</td>
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<td>0</td>
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<td>90</td>
<td>58</td>
<td>0.9</td>
<td>35</td>
<td>71</td>
</tr>
<tr>
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<td>0</td>
<td>0</td>
<td>144</td>
<td>0.4</td>
<td>19</td>
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</tr>
<tr>
<td>3a</td>
<td>Mixed</td>
<td>66</td>
<td>70</td>
<td>49.5</td>
<td>0.5</td>
<td>81</td>
<td>47</td>
</tr>
<tr>
<td>3b</td>
<td>Mixed</td>
<td>90</td>
<td>50</td>
<td>49.5</td>
<td>0.5</td>
<td>81</td>
<td>47</td>
</tr>
<tr>
<td>3c</td>
<td>Edge</td>
<td>90</td>
<td>144</td>
<td>49.5</td>
<td>0.5</td>
<td>81</td>
<td>47</td>
</tr>
<tr>
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<td>70</td>
<td>50</td>
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<td>0.4</td>
<td>77</td>
<td>100</td>
<td>0</td>
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<td>4b</td>
<td>Edge</td>
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<td>90</td>
<td>0.7</td>
<td>85</td>
<td>89</td>
<td>0</td>
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<tr>
<td>4c</td>
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<td>75</td>
<td>49.5</td>
<td>49.5</td>
<td>0.5</td>
<td>81</td>
<td>47</td>
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<td>5a</td>
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<td>69.5</td>
<td>49.5</td>
<td>0.5</td>
<td>81</td>
<td>47</td>
</tr>
<tr>
<td>5b</td>
<td>Edge</td>
<td>90</td>
<td>135</td>
<td>90</td>
<td>0.7</td>
<td>103</td>
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<td>47</td>
<td>47</td>
<td>0.9</td>
<td>82</td>
<td>68</td>
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<tr>
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<td>90</td>
<td>144</td>
<td>47</td>
<td>0.9</td>
<td>118</td>
<td>0</td>
</tr>
</tbody>
</table>

*Values of $\Delta W/10^{10}$ Nm$^{-2}$ are normalized to the sharpest minimum in the set (type 3b dislocations).

The energy factor $K$ was calculated using the linear anisotropic elastic theory of straight dislocations developed by Eshelby, Read & Shockley (1953) and detailed by Hirth & Lothe (1968). For a given $b$ the term in $R/r_0$ (typically $\sim 1.3$) is independent of the line direction and the preferred line direction for a dislocation can then be obtained from the condition that

$$\frac{K}{\cos \alpha}$$

is a minimum.

In order to find the position of this minimum for a particular dislocation, the dependence of $K/\cos \alpha$ on the line direction has to be determined.

The energy factor $K$ was calculated using the linear anisotropic elastic theory of straight dislocations developed by Eshelby, Read & Shockley (1953) and detailed by Hirth & Lothe (1968). In the general case of anisotropy, since $K$ cannot be expressed analytically, calculations were carried out numerically with the aid of a computer using Klapper's program DISLOC (Klapper 1972). The following values of the elastic constants (in GPa) for PETN were used in the calculation (Morris, 1976):

$$C_{11} = 17.18; C_{12} = 5.43; C_{13} = 7.48; C_{33} = 12.44; C_{44} = 5.03; C_{66} = 3.93.$$  

The results of the calculations are shown in Table 2. The calculated line directions are defined by two coordinates: $\theta$ and $\varphi$. $\theta$ is the angle between the dislocation and [001] while $\varphi$ is the angle between [010] and the projection of the dislocation line in the (001) plane. The term $\Delta W$ is a qualitative indication of the sharpness of the dislocation energy minimum, normalized to the sharpest minimum (type 3b dislocation, see Table 2) as unity, i.e. the sharper the energy minimum, the greater the probability that the observed line direction will lie along the direction of minimum energy. These results define the sixteen theoretically possible growth dislocation families that may exist in PETN. Each preferred line direction is representative of its dislocation family and all symmetrically equivalent line directions can easily be deduced from each unique configuration. The results of this analysis are summarized in Table 2.

3. Experimental characterization of dislocation configurations

3.1. Preparation of samples for X-ray topography

Crystals of PETN were grown from acetone and from ethyl acetate solutions by slow solvent evaporation and by temperature lowering (Hooper, McArdle, Narang & Sherwood, 1980). These crystals were typically $30 \times 10 \times 10$ mm and exhibited the forms $\{110\}$ and $\{101\}$ with the former dominant. The growth and perfection of PETN crystals is discussed in detail elsewhere (Halfpenny et al., 1984a). The crystals were sectioned parallel to (110) using a solvent saw and the resulting slices polished on a solvent-soaked cloth to a thickness ($t$) of about 1 mm. Cyclohexanone was found to be the most effective solvent for both slicing and polishing.

3.2. X-ray topography

Transmission X-ray topographs were recorded on a Lang camera using Cu $K \alpha_1$ radiation ($0.154$ nm). For this wavelength the linear absorption coefficient, $\mu$, for PETN is $1.64$ mm$^{-1}$. Thus the product $\mu t$ was approximately 1.5. The images were recorded on Agfa Structurix D4 X-ray film.
Table 3. Observed dislocation types in PETN

<table>
<thead>
<tr>
<th>Type</th>
<th>b</th>
<th>Growth sector</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>[001]</td>
<td>{110}</td>
</tr>
<tr>
<td>1b</td>
<td>[001]</td>
<td>{101}</td>
</tr>
<tr>
<td>2a</td>
<td>&lt;100&gt;</td>
<td></td>
</tr>
<tr>
<td>2b</td>
<td>&lt;100&gt;</td>
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<tr>
<td>3c</td>
<td>&lt;101&gt;</td>
<td></td>
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<tr>
<td>4c</td>
<td>&lt;100&gt;</td>
<td></td>
</tr>
<tr>
<td>5a</td>
<td>&lt;111&gt;</td>
<td></td>
</tr>
<tr>
<td>5c</td>
<td>&lt;111&gt;</td>
<td></td>
</tr>
</tbody>
</table>

3.3. Characterization procedure

The selection of X-ray reflections for the dislocation characterization was guided by the need for both extinction contrast and definition of the dislocation line directions. In the former case reflections were chosen such that the product \( g \cdot b \) should be zero for each likely Burgers vector. For some dislocations, unambiguous characterization was possible on the basis of this information alone. When a dislocation became invisible in fewer than two reflections, the characterization was completed by comparison of the observed and calculated line directions. Suitable reflections were found to be of the 200, 020, 220, 211, 121 and 222 types. In assessing the line directions full account was taken of projection distortion.

4. Results of the dislocation characterization

Table 3 summarizes the predominant growth dislocation types observed and characterized in PETN. The reference numbers and letters refer to the dislocation types listed in Table 2. Eight examples (labelled A to G in the following figures) have been selected to illustrate this characterization. The geometry of the slice containing dislocations A to C and E to G is shown schematically in Fig. 1. Figs. 2(a)-(f) are X-ray topographs of this slice. Dislocation D is shown in Fig. 3. The observed and calculated dislocation line directions for the dislocations in various reflections are listed in Table 4. These examples comprise all dislocation types observed in a wide range of crystals examined.

We have subdivided these eight characterizations into three loose groupings. Firstly, we describe those dislocations that can be characterized completely by extinction contrast experiments. We show that the dislocation line directions are in full agreement with those theoretically predicted and thus verify the applicability of this theory to the analysis of growth-induced dislocations in PETN. Secondly, we combine extinction contrast experiments with analysis from preferred line directions in cases where characterization by the former technique did not provide an unambiguous characterization. Thirdly, we apply the theoretical predictions to the case of dislocations which offer no extinctions for analysis by contrast considerations. In addition to this we note the qualitative information that can be gained from the dislocation images without use of the theoretical results.

4.1. Characterization from extinction contrast experiments

Dislocation A. The dislocations labelled A in Fig. 1 lie in the (110) growth sector. They are normal to the (110) face, which indicates they are probably pure edge or pure screw in character. This information limits the possible Burgers vectors to [001], [110], [111] or [111]. Beyond this, the dislocation line directions provide no further information. The dislocations are invisible in the 200, 020 and 220 reflections. The only Burgers vector that satisfies the condition \( g \cdot b = 0 \) for each of these diffraction vectors is [001]. Dislocations A are thus characterized as type 1a (dislocation types noted in this section refer to Table 2) with Burgers vector [001] in the (110) growth sector and are therefore pure edge in character.

Dislocation B. Dislocation B is in the (101) growth sector. Since it is not parallel to the growth direction it is probably mixed in character. It is also relatively...
Table 4. Observed and calculated line directions of dislocations A to G

<table>
<thead>
<tr>
<th>Dislocation Reflection</th>
<th>A 1a</th>
<th>B 1b</th>
<th>C 2a</th>
<th>D 2b</th>
<th>E 3c</th>
<th>F 4a</th>
<th>G2 5a</th>
<th>G1 5c</th>
</tr>
</thead>
<tbody>
<tr>
<td>220</td>
<td>Obs</td>
<td>Calc</td>
<td>Obs</td>
<td>Calc</td>
<td>Obs</td>
<td>Calc</td>
<td>Obs</td>
<td>Calc</td>
</tr>
<tr>
<td>220</td>
<td>90</td>
<td>90</td>
<td>156</td>
<td>88</td>
<td>90</td>
<td>57</td>
<td>38</td>
<td>60</td>
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<tr>
<td>12T</td>
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<tr>
<td>200</td>
<td>-</td>
<td>-</td>
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<td>-</td>
<td>-</td>
<td>33</td>
<td>33</td>
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<tr>
<td>002</td>
<td>95</td>
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<td>88</td>
<td>-</td>
<td>-</td>
<td>33</td>
<td>33</td>
</tr>
</tbody>
</table>
| Observed values refer to the projected angle \( \theta \) of the dislocation types specified in Table 2.

Fig. 2. Transmission X-ray topographs of crystal 1. The diffraction geometry, in each case, is shown in the inset. The reflections are: (a) 220; (b) 020; (c) 200; (d) 211; (e) 211; (f) 222.
Dislocation E. Dislocation E in Fig. 1 is relatively long, which suggests that it lies parallel to or at only a low angle to the slice plane. This, together with its projected line direction, shows that it is not parallel to the growth direction and is again of mixed character. The dislocation is invisible in both the 121 and 222 reflections. The only Burgers vector satisfying the condition \( \mathbf{g} \cdot \mathbf{b} = 0 \) in both cases is [101]. The observed and calculated line directions for this Burgers vector in the (011) growth sector also give good agreement as shown in Table 4. Dislocation E is therefore characterized as type 3c with Burgers vector [101] in the (011) growth sector.

4.2. Characterization from a combination of both extinction contrast and preferred line directions

Dislocation C. Dislocation C has the same projected line direction as A in many of the reflections. In the highly asymmetric 211 reflection, however, the difference in their true line directions is defined. Since A and C lie in the same growth sector and have different line directions, it follows that their Burgers vectors are different. As dislocation C does not lie parallel to the growth direction, it is probably mixed. It is invisible in the 020 reflection only. The Burgers vectors consistent with this result are [001], [100], [101] and [011]. [001] is eliminated by the argument above (i.e. it is not A). The dislocation is therefore characterized as type 2a with a Burgers vector [100] and lies in the (110) growth sector.

Dislocation G. Dislocation G exhibits a sharp change in line direction as it passes from the (101) to the (110) growth sector. Its Burgers vector must remain the same, however. Both parts of the dislocation \( G_1 \) and \( G_2 \) in the (101) and (110) sectors, respectively, are mixed since they do not lie along the growth normal in either case. The dislocation is invisible in the 211 reflection only. Its Burgers vector may therefore be either [111] or [011]. Only [111] gives good agreement between observed and calculated line directions for both growth sectors. Dislocation G is therefore of type 5a in the (110) sector (\( G_2 \)) and of type 5c in the (101) sector (\( G_1 \)).

4.3. Characterization from only the preferred line direction

Dislocation D. Dislocation D in Fig. 3 makes a large angle with the growth direction of the (101) growth sector in which it lies. It is therefore of mixed character. It did not become invisible in any reflection and consequently could not be characterized by the \( \mathbf{g} \cdot \mathbf{b} \) criterion. Examination of the calculated line directions for the (101) growth sector showed that only the Burgers vector [100] gave a line direction even remotely near to that observed. This Burgers vector gives good agreement between observed (\( \theta = 60^\circ \)) and calculated (\( \theta = 57^\circ \)) line directions. Dislocation D is therefore characterized as type 2b with Burgers vector [100] in the (101) sector and is of mixed character. It is noteworthy that no information about the Burgers vector of this dislocation could have been obtained without the calculated line direction.

Dislocation F. The dislocations labelled F have the same projected line direction as E in the 220 reflection. Their shorter length, however, suggests that they lie at a larger angle to the slice plane than the latter. The difference in projected line directions in other reflections confirms this. As discussed earlier, since they lie in the same growth sector, dislocations E and F must therefore have different Burgers vectors. Dislocations F remain visible in all accessible reflections, which again precludes characterization by the invisibility criteria. Comparison of observed and calculated line directions gives good agreement for a Burgers vector of [110] (type 4c) in the (011) growth sector. They are of mixed character.

5. Discussion

5.1. Basic growth-induced dislocation structure

The number of dislocations of each type within different samples was found to vary considerably with the crystal perfection. Consequently, the relative frequency of occurrence of each type can only be discussed in very general terms. From the twenty crystals examined, however, the following observations became apparent. Firstly, dislocations of types 1b, 2b, 3c, 4c and 5c, i.e. all those occurring in \( \{101\} \)
growth sectors, were less common than the remaining types. The crystal slice shown in Fig. 3 is almost devoid of dislocations in one of the \{101\} sectors. Where dislocations occurred in large numbers in these sectors, however, those of types \(3c\) and \(5c\) were usually dominant. Of the dislocations occurring in \{110\} sectors, those of type \(5a\) were by far the most common with type \(1a\) dislocations also present in significant numbers.

It is interesting to recall that growth dislocations in PETN have been observed having Burgers vectors up to and including \{111\}. No evidence has been found for dislocations of larger Burgers vectors. The elastic line energies of those observed range from 19 to 83 eV nm\(^{-1}\). The growth dislocations are clearly not confined to those of lowest line energy. In fact, the most commonly occurring dislocation type is that of highest line energy. Dislocations with large line energies have also recently been observed in single crystals of ammonium dihydrogen orthophosphate (Bhat, Roberts & Sherwood, 1983). These observations suggest that the line energy of a given dislocation is not necessarily the controlling factor in determining whether or not the dislocation occurs.

Bearing in mind the manner in which growth dislocations are formed, i.e. at inclusions or at disturbed regions of the crystal such as the seed, the most significant factor in determining the Burgers vector is probably the nature of the misorientation at which the dislocation is nucleated.

### 5.2. Dislocation motion and mechanically induced dislocations

It is interesting to note that the dislocations observed in PETN exhibited an almost exclusive linear line direction with no evidence for dislocation motion either during or after growth. Etching and micro-hardness indentation studies of PETN (Halfpenny, Roberts & Sherwood, 1984b) have shown that the material is comparatively soft (surface hardness 17 kg m\(^{-2}\)) and readily undergoes slip on the \{110\} planes. The lack of glide-induced motion of most growth dislocations could be explained by their potential sessile nature (with the exception of type \(1a\)), i.e. the fact that \(l\) and \(b\) do not lie in the dominant \{110\} slip planes. In contrast, dislocations of type \(1a\) (edge type \(l\parallel[110], b\parallel[001]\)) certainly should slip. That they do not do so could reflect the fact that rather low mechanical stresses develop in the crystals during growth.

A further observation which could also explain the lack of motion is our difficulty in obtaining extinction conditions for dislocations in this material. This could well reflect a high level of impurity or, more probably, solvent decoration of dislocations. In addition to causing the observed effect, this could also result in dislocation pinning and hence restriction of migration by either slip or climb. We believe that either of these possibilities could perhaps explain the lack of dislocation motion in this solid.

### 6. Conclusions

This study shows the utility of Klapper's theory of preferred dislocation line directions as an aid in the provision of complete and comprehensive analysis of growth-induced dislocation structure in single crystals. Using, initially, a combination of extinction contrast criteria and preferred line directions we verify the applicability of this theory in the case of the energetic solid PETN. Latterly, we are thus able, on dislocation line direction data alone, to characterize many dislocations of mixed character whose Burgers vectors we cannot unambiguously define using extinction contrast criteria.

Eight families of dislocations with Burgers vectors \{001\}, \{100\}, \{101\}, \{110\} and \{111\} are observed in single crystals of PETN. Dislocations with the long Burgers vector \{111\} are found to predominate in the dislocation structure suggesting that the line energy is not the dominant factor in dislocation formation. All of the dislocation types, with one exception, which is an edge dislocation, are of mixed character. This solid exhibits no direct evidence for growth-induced dislocation motion by either glide or climb mechanisms. This we attributed to the mostly sessile nature of the dislocations observed, together with a likelihood of solvent-impurity pinning of the dislocations.

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### References


