The kinematics of deformation and the development of substructure in the particle deformation zone

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Abstract.
The details of the deformation near undeformable particles influence the recrystallization behaviour of commercial aluminium alloys. It has been shown that the size of the particle deformation zone (PDZ) and the local lattice rotation decrease with particle size and that a uniform distribution of very small closely spaced particles makes the deformation more homogeneous. Although a number of models have been proposed to describe the development of the PDZ, an explanation for this particle size effect remains elusive. In this paper, high resolution digital image correlation was used to map the deformation around particles of different sizes in a model Al-Si alloy. Deformation maps were compared to maps of local lattice rotation obtained using electron back scattered diffraction (EBSD) to elucidate the link between the kinematics and the resultant substructure. These results were also compared to crystal plasticity finite element predictions. The deformation maps revealed that deformation is concentrated in intense slip bands that have a characteristic spacing and which are strongly correlated to the deformation substructure. Whereas particles larger than this characteristic spacing interact strongly with the slip bands, causing large local rotations, smaller particles either interact more weakly or not at all. Since the strain between the bands is only a fraction of that in the bands, the rotations associated with the smaller particles are invariably smaller. Very small, closely spaced particles change the slip band pattern, decreasing the band spacing and decreasing the amount of shear within the bands. CFEM modelling was able to reproduce general features of the particle deformation zone but because it does not predict the development of slip bands and their characteristic spacing it fails to predict an effect of size on the local rotation.

1. Introduction
The microstructure of aluminium alloy products is determined during thermomechanical processing. The processing parameters are controlled to produce the grain size and texture required by the application. Deformation breaks down the cast structure and provides the driving force for subsequent recrystallization during annealing. Almost all commercial alloys contain second phases of varying sizes and origins, which are well known to affect the development of the deformed state and the recrystallisation behaviour during annealing [1]. Small, closely spaced particles <1 µm are known to retard and hinder recrystallization [2], whereas larger particles can stimulate the nucleation of new grains during recrystallization, which helps to refine the grain size and also randomise the texture, which is important to reduce the anisotropy of the final product [1]. The stimulating effect of large particles originates from the formation of a particle deformation zone (PDZ) in the matrix near the second phase particles, where the deformation is different from that in the bulk. This difference gives rise to highly misoriented
regions within the PDZ, which act as preferential nucleation sites during recrystallization. The local misorientation was studied extensively by Humphreys and collaborators using both TEM and X-ray diffraction on single crystals [3, 4] and later using electron backscattered diffraction (EBSD) on single crystal [5] and polycrystalline samples [6, 7]. They found that the amount of rotation in the PDZ in a single crystal increased with particle size with the rotation near a $4\mu m$ being almost twice that near a $1\mu m$ particle. Beyond a particle size of $3-4\mu m$ the amount of rotation remains essentially unchanged. In polycrystalline material, the measured local rotations are smaller [4] and show a considerable amount of scatter [6]. When the particles are very small, of the order of $100\ nm$, evenly dispersed and closely spaced, not only are the PDZ and associated rotations very small, the deformation is generally more homogeneous and intergranular misorientations are reduced throughout the material [7, 8].

A number of models have been proposed to explain the formation of the PDZ and associated lattice rotations. Early models focused on how the misfit between the matrix and the deformable particles could be accommodated by dislocation generation and dynamic recovery [9, 3] but this treatment is only applicable to small strains. Later models attempted to explain how the presence of the particle affects local plasticity using Taylor multislip modelling [4, 5] and more recently crystal plasticity finite element (CPFE) modelling [10, 7]. CPFE models successfully predict the general shape of the PDZ around large particles, with good agreement with measured local lattice rotations for single crystals. They also predict that the shape and extent of the deformation zones around particles depends on the initial grain orientation, which implies that the PSN effect will depend on the orientation of the grain in which it develops. However these models cannot capture the effect of particle size on the lattice rotation in the PDZ, even when using strain gradient plasticity to introduce a natural lengthscale [10], and fail to explain the large scatter in local lattice rotation measured in polycrystals [6], which could be related to the low efficiency of PSN. These models also cannot explain why very small closely spaced particles homogenise the deformation structure [8, 7].

One of the difficulties in understanding the limitations of current models is that comparisons with experimental data are limited to lattice rotation data. This is problematic for two reasons. Firstly, modelling predictions are different for different starting grain orientations but experimentally, the starting orientation of a grain is usually not known. Secondly, the lattice curvature measured using EBSD or TEM does not uniquely determine the kinematics of the deformation because there is more than one possible strain distribution that is compatible with a given lattice curvature and therefore agreement between the lattice rotation predicted by a crystal plasticity model does not fully validate the model. One way to address these difficulties is to measure directly the strain distribution around the particle as well as the lattice rotation in a grain with known starting orientation.

In this work, high resolution digital image correlation (HRDIC) [11] was used to map the kinematics of deformation around particles of different sizes in a model Al-Si alloy during deformation in plane strain compression. EBSD was used to determine the orientation of the matrix before deformation and to map the local lattice rotation after deformation. The experimental results were also compared with predictions from a CPFE simulation using an image based mesh. The aim was to measure how the kinematics of deformation is affected by the particle size and to explain why and how continuum crystal plasticity models fail to predict these size effects.

2. Material and experimental procedure

2.1. Material

The material studied was a model Al-Si alloy which can be heat treated to precipitate particles of varying sizes. The chemical compositions of the alloy is given in table 1. The material was first solution heat treated at $580^\circ C$ for 6 hours and then water quenched. Two particle distributions
Table 1. Chemical composition of the model Al-Si alloy studied (wt%).

|   | Si  | Fe  | Cu  | Ti  | B   | Al   |
|---|-----|-----|-----|-----|-----|------|
|   | 0.81| 0.002 | 0.001 | 10.0003 | 0.0005 | Bal. |

Figure 1. SEM images of the starting microstructure of the alloy in the two conditions (a) following a prolonged heat treatment to give large, widely spaced particles (b) following solution heat treatment and low temperature heat treatment to precipitate small sub micron sized particles.

were then produced by ageing: large, widely spaced particles were generated by heat treating at 490 °C for 120 hours, followed by slowly cooling at 1 °C/h to room temperature, and very small, closely spaced particles by heat treating the material at 200 °C for 90 minutes, which is part of the gold remodelling procedure required for the strain mapping. The two microstructures produced are shown in figure 1. The material containing coarser particles shows range of particle sizes at a range of distances with an average particle size of 10 µm, which at volume fraction of 0.8% corresponds to an average distance between particles of 23 µm. However, there is a preference for precipitation at the grain boundaries and therefore inside the grains the interparticle spacing is larger. The second heat treatment produces evenly spaced small particles ranging in size from 100 to 200 nm with an average spacing of 1-2 µm spacing. The grain size was about 1 mm in both materials.

After heat treatment the samples were machined into 5×5×5 mm cubes for testing using a diamond saw. The surfaces to be studied were then polished using diamond paste of size 6, 3 and 1 µm, followed by 30 minutes of OPS polishing to achieve a shiny, deformation free surface ready for EBSD.

2.2. EBSD
EBSD was used to map the starting orientations of the grains before deformation and to map the lattice rotations after deformation. For the initial maps, 2 × 2 mm areas were mapped with a 2 µm step size in the centres of the compression samples, using a CamScan Maxim FEGSEM operating at an accelerating voltage of 20 kV controlled via the HKL Channel5 software from Oxford Instruments. These maps were also used to select areas of interest for the deformation
mapping.

The maps after deformation were made with a much smaller step size of 0.1 μm, which is similar to the spatial resolution of the deformation mapping measurements, using a Magellan XHR FEGSEM operating at an accelerating voltage of 20 kV and also controlled via the HKL Channel5 software from Oxford Instruments. These final EBSD maps had indexing rates of around 95%. Non-indexed pixels were extrapolated using the neighbour orientation using the Channel 5 software. Then the data was filtered with two passes of a Kuwahara filter with 5x5 pixel block as implemented in VMAP, which allows misorientations as small as 0.5° to be detected [12]. The region of interested was also imaged using electron channelling contrast imaging (ECCI) after deformation to reveal the deformation substructure using a Magellan XHR FEGSEM at 15 kV with a working distance of 5 mm.

2.3. Deformation mapping

After EBSD, the samples were prepared for the HRDIC measurements using the procedure described by Di Gioacchino and Fonseca [11]. This involves coating the polished surfaces with a thin layer of gold (~ 50 nm) using an Edwards S150B sputter coater. This surface layer is then remodelled by placing it in a water vapour environment at 200°C for 90 minutes. This produces a fine, uniform, characteristic distribution of gold speckles on the surface, which makes it possible to map local strains with 0.1 μm resolution using digital image correlation.

The samples were compressed at room temperature using an Instron 5569 testing machine using a channel die to simulate plane strain compression (PSC) as shown in figure 2. Two cubes, each with a surface prepared using the gold remodelling procedure, were placed in the die with the surface of interest normal to the transverse direction. A thin (40 μm) PTFE film was placed between the cubes for lubrication. Each loading step had a target strain of 5%. Since the required displacement was very small (≤0.25 mm), the crosshead movement was not a good indicator of the strain in the sample and, in some cases, 2-3 attempts were needed to obtain a 5% reduction. After each 5% increment, the cubes were removed from the die, separated and imaged. These experiments were limited to a reduction of 30% because further compression damaged the gold pattern beyond use.

A high resolution Scanning Electron Microscope (Sirion FEGSEM) was used for backscattered electron imaging of the regions of interest. The imaging conditions were optimised for Z-contrast, so the gold particles appear bright and the aluminium background appears dark, in low contrast with the silicon particles. The working distance was kept low at 5 mm to maximise the BSE
signal. An 8 bit depth was used during imaging. After each strain increment, the sample was placed in the microscope and the image was focused ensuring that the working distance was maintained constant at exactly 5 mm. A magnification of 2000× was chosen so that each gold spot covers at least 3×3 pixels. The sample is always aligned with the bottom edge, which is parallel to the rolling direction during deformation.

After acquisition, the images were processed using the software Davis, from LAVision, Gottingen. The image correlation uses an adaptive multipass FFT implementation, where the search window is shifted and deformed iteratively by displacements of the neighbouring windows as described in [13]. The initial window size used is 512×512 pixels with an overlap of 50%. This is incrementally halved until a final window size of 8×8 pixels, at which 3 iterations are performed. The final overlap between windows is 50%. A circular Gaussian weighting window is used at the final size, which slightly improves the signal to noise ratio of the image correlation.

Digital image correlation gives maps of displacement from which the in-plane compressive axial strain, $\epsilon_{yy}$, and the in-plane rotation, $\omega_z$, can be calculated:

$$\epsilon_{yy} = \ln(1 + \frac{dv}{dy})$$

$$\omega_z = \frac{1}{2} \left( \frac{du}{dy} - \frac{dv}{dx} \right)$$

where $du$ and $dv$ are the displacements along $x$ (RD) and $y$ (ND) respectively.

3. Results

Sequential images were acquired at a large number of different locations, sampling different grain orientations, however due to space constraints only the results of three representative regions are shown here for the material containing coarse particles: a region containing no particles, a region containing a large (>10 $\mu$m) particle and another containing a smaller (<2.5 $\mu$m) particle. For the material containing very fine (100 nm to 200 nm) particles, the results from only one representative region are presented. All deformation maps are presented in the deformed configuration.

3.1. Deformation away from particles

In the material with coarse particles, the average distance between particles is about 50 $\mu$m and therefore in much of the material deformation occurs away from the influence of particles and is representative of the deformation of the pure metal [3]. Images of the gold remodelled surface in a region without particles are shown, at different deformation levels, in figure 3. The figure shows a region within one grain where the gold remodelling process produced, fortuitously, a straight boundary separating slightly different speckle morphologies. The deformation is concentrated on thin bands of slip, separated by regions with much less strain. As can be seen by the relative movement of the circled gold speckles, the distance between the top and middle circles decreases much more quickly than that between the middle and bottom one, which remains almost constant during deformation. This difference is caused by the larger number of slip bands on the top half of the region imaged. Before deformation starts, the boundary separating the two speckle regions is parallel to the compression axis. During compression, the material lattice starts to deform and the speckle boundary is sheared and broken up by the appearance of slip bands. As the boundary is broken up, it starts to rotate anti-clockwise as do the slip bands. This rotation is clearly not uniform and appears to be related to the different amounts of shear in the different bands.

This deformation heterogeneity can be quantified using HRDIC. The axial strain ($\epsilon_{yy}$) maps for this region are shown in figure 4. There are two sets of maps, each showing the strain after
Figure 3. A small region within one grain far from any particles or grain boundaries imaged at different strain levels (a) 0% - a straight boundary between two regions of the surface where the speckle pattern in slightly different (b) after 16% strain the boundary is broken by a series of intense slip bands with the segments rotating to different extents (c) after 30% compression the boundary is broken down even further and becomes more diffuse. The top of the region has clearly deformed more that the bottom as the relative movements of the circles indicate.

11%, 16% and 30%. In the first one, shown in figures 4 (a) - (c) the maps show the increments of strain between successive images whereas in the second, shown in figures 4 (d) - (f) they show the total strain.

The strain maps show clearly that the number of slip bands increases slightly with strain, with a secondary set of bands, which are perpendicular to the primary set, appearing at the 16% strain increment. When new primary band A appears at 16% strain, it seems to inhibit slip in the neighbouring band B. The increase in the number of bands makes the bands in the total strain map (figure 4) appear to broaden. The primary slip bands are aligned at 30° to the rolling direction after a reduction of 11% and rotate towards RD with increasing strain, approaching 15° after a reduction of 30%. Although the slip bands are approximately parallel, this alignment is clearly not perfect: the bands are not straight, and new bands that appear later in the deformation are at a higher angle to the existent bands. This is particularly clear in figure 4 (c). The plot in figure 5 shows the strain along the line marked in figures 3 (c) and 4 f. The plot confirms that deformation occurs mainly in the slip bands with the matrix between the bands deforming much less. The strain in the regions between the slip bands appears to increase at 30% applied strain but it is clear from figure 4 (c) that this increase in strain is caused by an increase in the number of bands parallel to the primary bands and the appearance of complementary secondary bands. It is not possible to generalise from observations of a single, small region, but by repeating this analysis over several different regions the following generalisations can be made. The deformation of the matrix away from the particles and grain boundaries is very heterogeneous, with most of the strain being born by almost discrete slip bands which are about 100 nm thick and which effectively broaden with deformation by the activation of new parallel bands. The spacing of the slip bands ranges from 3 to 4 µm irrespective of grain orientation and decreases only slightly with deformation. Although the primary bands in the region presented here start off at 30°, the initial alignment of slip bands is usually closer to 45° but soon develops a different preferential alignment, which sometimes coincides with {111} slip traces but usually does not. At very low strains (≤ 5%) there are usually two sets of weak slip bands with opposite shears (not shown here) and one of these soon dominates to become the primary set, as shown in figure 4, up until a strain of 0.2 to 0.25 when a second complementary set reappears, not usually
Figure 4. Axial compressive strain maps for a region away from any particles and away from a grain boundary after overall compression by 11%, 16% and 30%. (a)-(c) show the increment in strain between successive deformation steps, which are indicated below the images. (d)-(f) show the total strain at the 3 increments.

Figure 5. Compressive axial strain profiles along the line marked in figure 4 (f). The profiles are aligned with the bottom slip band, with the corresponding peaks marked with an arrow.
aligned with slip traces. After 30% reduction the average strain accumulated between the slip bands is about 0.2, whereas the strain in the bands is about 1.5 and can be as high as 3. Thus, although the slip bands are much narrower that the distance between them, they still account for the majority of the deformation at 30% applied strain. The alignment of the dominant bands is clearly dependent on crystal orientation, although orientation is not the defining criterion. In fact, some grains show different slip band alignment in different parts of the grains. For near stable orientations, slip bands are fairly straight and tend to align between $\pm 30^\circ$ and $\pm 40^\circ$. For more unstable orientations, the slip bands are less straight and therefore show a greater range of alignment angles.

3.2. Deformation near an isolated 10 $\mu$m particle

3.2.1. Deformation mapping

An example of the development of strain and material rotation during plastic deformation in the matrix around a large particle is shown in figure 6 for a grain with near cube orientation ($\phi_1 =80^\circ$, $\Phi =14^\circ$, $\phi_2 =9^\circ$). As can be seen, both strain and rotation are mainly concentrated along primary slip bands. At the beginning of deformation (average strain in the region of 0.08) the local strain is around 0.5-0.8 in slip bands, up to 10\times the applied strain. In contrast, the strain in areas between slip bands is only around 0.05, slightly less than the applied strain. When the strain increases to 0.2 and 0.3, the strain in the slip bands increases to almost 1 and new slip bands appear, including a second set at around 0.25 strain. This shows that the pattern of deformation near a particle is, in general terms, very similar to the deformation away from the particle. However the presence of the particle changes the details of the pattern in the regions near the particle.

The first obvious effect is that the particle interrupts intersecting primary slip bands from the start of deformation. Interrupted bands are indicated by arrows in figure 6 (a), (c) and (e). The bands are not interrupted at the particle but at some distance away from it, approximately equal to the particle size. The presence of the particle also appears to cause some of these primary slip bands to bend. A good example is the band that propagates from the interrupted band above and to the left of the particle. This bending occurs at very low strains and therefore is not caused by local lattice distortions. This also implies that the bands are not crystallographically aligned. The third effect is an increase in the density of slip bands in the regions near the sides of the particle which are parallel to the slip bands. In this case, the particle increases the density of both the primary bands, especially below the particle and at larger deformations that of the secondary bands, to the left and right of the particle. Interestingly one secondary band seems to be nearly continuous across the particle and is not interrupted like the primary bands were.

The HRDIC maps in figure 6 (b), (d) and (f) show that rotation is also concentrated in the bands, which implies that deformation in the bands occurs by unidirectional shear. However, it is also seen that the rotation in the regions between the bands, where there is much less shear, is not homogeneous. At $\epsilon_T = 0.08$, a $-5^\circ$ rotation (a negative rotation is anti-clockwise here) can be seen at the top left and bottom right corner of the particle (b). With an increase in strain to 0.2, there is a global rotation of $-5^\circ$ of the entire area and the rotation around the particle increases to $-10^\circ$ in parts of (b). When the strain further increases, both positive and negative rotations around different sides of the particle can be seen. At an applied strain of 0.3, the regions near the particle have rotated to $5^\circ$ and $-15^\circ$.

3.2.2. Lattice rotation mapping

Figure 7 shows the EBSD derived local lattice rotations of the region mapped in 6 relative to a point near the particle, marked with a *, where the material has remained undeformed. The maximum misorientation measured is lower than that measured in single crystals [3] but is in better agreement with more recent EBSD measurements in polycrystals [7]. The maps show the amount of lattice rotation around the RD (x), TD (y) and ND (z) axes, where a positive angle represents a clockwise rotation. The rotations are
Figure 6. Maps of the local deformation around a large particle measured using HRDIC. Axial strain, $\epsilon_{yy}$, is mapped in (a), (c) and (e), and the rotation, $\omega_z$ is mapped in (b), (d) and (f). Note that $\epsilon_T$ is the total strain in the area mapped.
largest around TD but are non-zero around RD and ND. This implies that although the imposed deformation is plane strain, the resultant lattice rotations are 3 dimensional. The particle clearly affects the local lattice rotation, forming the typical pattern of rotations associated with the particle deformation zones observed in aluminium alloys. A region of negative TD rotation of about $-10^\circ$ can be seen at the upper left and lower right corners whilst a region of positive rotation exists in the upper right and lower left corners of the particle, of around $3^\circ$ and $10^\circ$ respectively. These regions have sizes comparable to that of the particle and are remarkably similar both in shape and magnitude to the material rotations in the regions between the bands in figure 6 (f). In addition, there are some very localised 1-2 $\mu$m regions of high positive local lattice rotation at the bottom of the particle. These seem to be directly related to very local changes in the thickness and direction of the slip bands.

3.3. Deformation near an isolated 2$\mu$m particle

3.3.1. Deformation mapping The deformation maps for a region containing a smaller 2 $\mu$m particle are shown in figure 8. The orientation of the grain containing this particle is different ($\phi_1 = 4^\circ$, $\Phi = 40^\circ$, $\phi_2 = 26^\circ$) and, as a consequence, the evolution of deformation heterogeneity is also slightly different demonstrating that although the alignment of slip bands is not crystallographic, it is orientation dependent. Although these maps were obtained at the
same strain increments as for the large particle, the local strain in this region is about half, demonstrating the large variations in local strain possible in a polycrystalline material. As before, most of the deformation occurs by shear in discrete slip bands. However, in this case, the second set of slip bands is already visible after an average strain (for the region) of just 0.04 and well established at 0.10. It is worth noting, however, that presumably because this is a harder grain, the macroscopic strain is about twice as high and therefore these secondary bands appear at the same macroscopic strain increment as they did near the larger particle. The number of slip bands increases progressively with deformation and the distance between them

Figure 8. Maps of the local deformation around a small particle measured by HRDIC. Axial strain is mapped in (a), (c) and (e), and the rotation is mapped in (b),(d) and (f). Note that $\epsilon_T$ is the total strain in the area mapped. The actual applied strain is about twice $\epsilon_T$. 
decreases accordingly. However, the spacing of slip bands is always larger than the particle size. Unlike in the case of the large particle there is no obvious effect of the presence of the particle on the deformation around it. However the distribution of slip bands varies across the region, with a slightly higher density of slip bands just to the right of the particle, for example. At $\epsilon_T = 0.16$ there are two clear sets of complementary bands everywhere apart from the top right region, where the primary bands dominate.

The rotation maps show that the region first rotates homogeneously clockwise by up to $2^\circ$, and then splits up, with the central region rotating to about $-6^\circ$ and the top right region, where the primary bands dominate, rotates to $7^\circ$. As in the strain maps, the presence of the particle does not seem to affect the local rotation. Rather, it seems to be affected by the intensity, density and spacing of the slip bands which varies with position independently of the presence of the particle.

3.3.2. Lattice rotation mapping Figure 9 shows the local lattice rotation maps obtained by EBSD for the same region. As with the large particle, the change in lattice rotation is highest around TD, but in this case both the ND and RD show considerable orientation gradients of over $10^\circ$. However, the highest gradients are not associated with the particle. Instead they appear to delimitate regions far from the particle where the slip band characteristics are different. Around
Figure 10. Maps of the local deformation in a material containing very small, evenly spaced particles measured by HRDIC. Axial strain is mapped in (a), (c) and (e), and the rotation is mapped in (b),(d) and (f). Note that $\epsilon_T$ is the total strain in the area mapped.

TD, the biggest gradient is at the top of the image, towards the right, which corresponds to the region where only primary bands can be seen in the strain maps in figure 8 (e). Again the lattice rotations are very similar to the material rotations in the regions between the slip bands although in this case the changes in material rotation cannot be related to the particle. In fact there is a strong correspondence between the slip bands and the lattice rotation maps, with features at the top well aligned with the primary deformation bands and those at the bottom aligned with the secondary bands.
3.4. Deformation in the presence of closely spaced, small (< 200 nm) particles

3.4.1. Deformation mapping  Forgoing the ageing heat treatment causes the gold remodelling procedure to precipitate very small particles about 100 to 200 nm in size with 1 to 2 μm spacing. Figure 10 shows the deformation in this material, in a grain with orientation $\phi_1 = 31^\circ, \Phi = 1^\circ, \phi_2 = 72^\circ$. Deformation is clearly still dominated by the appearance of slip bands but these have a significantly smaller spacing of about 1 to 2 μm, identical to the interparticle spacing. Unlike in the material with coarse particles, the amount of strain within the bands varies noticeably along their length. In fact the bands often appear to be interrupted and slightly offset. Careful examination of the strain maps and the source images reveals that these interruptions and the associated variations in strain are associated with the presence of particles. At a mean strain of 0.12, the strain in slip bands varies from 0.1 to 0.8, with an average of 0.4. At a mean strain of 0.3, this increases to 0.653. In between the bands, the strain varies from 0.03 - 0.07 at $\epsilon_T = 0.12$ and between 0.12 - 0.17 at $\epsilon_T = 0.3$. As was the case in the aged material, secondary slip bands appear at a strain of 0.25 but they are much less intense and much more closely spaced. Clearly the presence of closely spaced small particles makes the deformation much more homogeneous.

The material rotation ($\omega_z$) maps in figures 10 (b), (d) and (f) show that the the rotation of the regions between the primary slip bands starts out very homogeneously. However, with deformation, a patchwork of regions several μm in size with rotations ranging from 0 to 15° develop. However, careful observation reveals that these regions do not correspond to rigid body rotations like those found in the material with coarse particles. Instead they originate from the shear in closely spaced secondary slip bands.
3.4.2. Lattice rotation mapping  
Figure 11 shows the EBSD result in the centre of the region mapped in figure 10. A smaller subregion was mapped at a higher magnification to reveal the subtle substructure that emerges in this case. The lattice rotation maps reveal patches of alternate lattice rotations 4 - 6 µm in size that correspond to the patches of material rotation identified in the DIC rotation maps. However the misorientations between patches are very small, with a maximum of 2.5°. Some patches are separated by segments of low angle grain boundary, as shown by the misorientation profile in 11 (e). This means that although the shape of the patches is similar in both maps, the amount of lattice rotation between the bands is much smaller than the amount of material rotation measured, unlike in the material containing coarse particles where the two were very similar.

4. Discussion
4.1. The kinematics of deformation and local lattice rotation
The HRDIC measurements have revealed that the deformation in the absence of particles is heterogeneous, with the formation of one set of primary slip bands at the start of deformation and the activation of complementary bands at higher strains. The occurrence of slip bands during deformation of aluminium and its alloys has long been recognised [14] but because these bands are narrow and sparse, their contribution to the overall deformation was assumed to be minimal. However, these new measurements demonstrate, unambiguously, that most of the deformation is in fact accommodated by shear in these bands. The bands have a characteristic spacing of 3-4 µm, which is comparable to the size of the cells formed in this material, suggesting there is a direct relationship between the slip bands and the low angle grain boundaries observed after deformation. The bands are not aligned with slip traces, implying multiple slip within bands, but their alignment does depend on the crystal orientation.

Although the imposed macroscopic deformation is plane strain compression, the local deformation in all the regions studied show significant shear and rigid body rotation. This implies that within a grain inside a polycrystal, the deformation constraints are somewhat relaxed with overall compatibility being achieved by heterogeneous deformation elsewhere in the grain or even in neighbouring grains. Paradoxically, this suggests that the deformation of a grain embedded in a polycrystal deforming in plane strain might be less constrained than a single crystal deformed in plane strain. The consequence is that for much of the deformation most of the shear occurs on one set of primary bands which causes large rotations of the grain, with a second set of complementary bands appearing only at a strain of about 0.25.

The presence of large particles affects the deformation by interacting locally with the slip band pattern. The stresses associated with the particle cause changes in the direction, width, intensity and number of slip bands in the particle deformation zone. This is consistent with the idea that the particle modifies the local plasticity by changing the local slip system activity, as proposed by Humphreys and Kalu [5]. However the details of the kinematics are quite different from those usually assumed. Whereas the in their model the deformation was assumed to be homogeneous with the particle shadowing slip in the different regions around the particle, these results show that in practice this is instead achieved by modifying the discrete slip band pattern that characterises deformation at this scale.

One remarkable observation is that the EBSD lattice rotations are almost identical to the HRDIC material rotations of the regions between the slip bands. This is unexpected, since in crystal plasticity material rotation and lattice rotation should not coincide. This is why the slip bands appear in the material rotation maps and not in the lattice rotation maps. However, because the strain between slip bands is much less that that in the bands, their rotation is determined by the shear in the slip bands and not by the local plastic strain. The stresses around the particle affect the intensity, width, spacing and direction of the slip bands changing the magnitude of the average local shear, and giving rise to the rotations in the PDZ around.
the particle, which extend out to about 1 particle diameter away from the interface. In addition to these rotation zones, there are also more localised lattice rotations associated directly with changes in the width and direction of the slip bands, which give rise to much smaller \( \sim 1 \mu m \) misoriented regions near the particle. This is a consequence of the multislip nature of the deformation in these bands, which are actually made up of a fine structure of nonaligned slip, as shown in figure 4 (f).

All these observations suggest that the development of the substructure is directly related to the heterogeneity of deformation. This relationship is confirmed in figure 12 where the region around the largest particle is shown in back scattered contrast alongside the rotation map from HRDIC, a misorientation map from EBSD and the lattice rotation around ND. The electron channelling contrast image shows substructural features aligned with the slip bands in the DIC map. This alignment is even clearer in the misorientation map shown in figure 12 (c) where low angle grain boundaries are outlined. There is direct correspondence between slip bands and low angle grain boundaries in many instances. Although not all slip bands have a corresponding low angle grain boundary, the thicker, more intense ones invariably do, especially those which are forced to bend by the presence of the particle. The regions close to the bottom right corner of the particle, where the slip bands are much closer are offset and also bifurcate, correspond to small subgrains, which were probably formed by the complex local deformation and the very high levels of shear strain associated with the slip bands. Not all bands are associated with subgrains. One such region is that under the green arrow in figure 12 (c), where there is an absence of low angle grain boundaries, even though there are clearly several slip bands. The most likely reason for the absence of low angle grain boundaries here is the lower magnitude of shear in these bands.
If the particle deformation zones are formed by the interaction of the particles with the slip band pattern, this offers an explanation for why the size of the PDZ and lattice rotation is smaller for smaller particles. As the deformation maps near the smaller particle exemplify (figure 9), when the particle size drops below the slip band spacing, the probability of a particle interacting with the slip band decreases and when it does, the effects will be smaller than with large particles. If the particle does not interact with a slip band then the effects will be even smaller because, although the deformation between bands is not zero, it is much less that the strain in the slip bands. The region near the small particle also shows how the lattice rotation generated away from particles by changes in the deformation pattern can be as large as that in a PDZ. The change in slip band alignment gives rise to misorientations of 15°, almost as large as those seen near the large particle. This behaviour is similar to that observed on cube oriented single crystals deformed in uniaxial compression by Liu and Hansen [15], and is therefore not limited to polycrystalline materials. The interaction of the particle with the deformation pattern will depend not only the particle size but also its shape and orientation with respect to the slip pattern and the characteristics of the deformation pattern will depend on grain orientation and local stresses within the grain, which in a polycrystalline sample is affected by neighbouring grain interactions. Taken together, these observations also imply that, in practice, there should be significant variability in the size of the PDZ and on the local misorientations generated, particularly for smaller particles. This is in agreement with previous measurements [6] and consistent with the randomization of texture associated with PSN.

The idea that heterogeneous deformation in the form of intense slip bands is essential to the formation of the deformation substructure can also explain the change in behaviour observed in the presence of very fine, closely spaced particles [8]. The results here show that small, closely spaced particles modify the deformation pattern, causing it to be more homogeneous. Discrete slip bands still appear but they are more closely spaced and less intense. Although as particles become smaller the mechanism of interaction between the particles and the deforming particle will change [16], another important consideration must be the distance between the particles. According to our results, the interaction between the deformation pattern and the particle should decrease as the particle size decreases. However, if as the particles become smaller they also become more numerous and more closely spaced, as often is the case, then interaction with the deformation pattern becomes unavoidable. In the material studied here, the particles are 1-2 µm apart and are about 100 nm in size. The end result is that every particle interacts and interrupts a slip band after only a few micrometres, forcing the slip band spacing to decrease. Deformation continues but at larger stresses, which, in combination with the much more homogenous slip allows local stress variations to be accommodated without significant large accompanying lattice rotations.

4.2. Comparisons with crystal plasticity finite element modelling

Crystal plasticity finite element modelling (CPFEM) was used used to model the deformation around the large particle. CPFEM is used for a variety of applications [17] including the modelling of deformation at the microstructural scale. The implementation used in this study was developed by Bate [18] and has been used to predict the formation of deformation bands and PDZ in both 2D [10] and 3D [7]. Although the same implementation is used the details of the model used here are quite different. In an attempt to capture any geometric effects of particle geometry, the mesh was created by sampling the EBSD map before deformation and using quadratic hexahedral elements to make up a volume which was 1 element thick, with the area mapped represented by an array of 70×95 elements. The boundary conditions were applied to simulate plane strain compression to a compressive strain of 0.3 in increments of 1×10⁻⁴. This model is clearly unrealistic in several ways. In practice, deformation will be 3 dimensional and the material around the particle is therefore over-constrained in the model.
This is particularly true for modelling the plane strain compression experiment because although the particle is constrained to some extent, a small amount of out of plane deformation can and does occur. However it is difficult to do much better without knowledge of the full shape of the particle and grain below the surface. This means that quantitative comparisons must be made with care and the impact of these shortcomings should be considered when comparing the results of the simulation with those of the experiment. The material model, the details of which can be found in [18], [10] and [7], was calibrated using both the stress-strain data from compression testing and plane-strain compression testing of the material containing coarse particles, with a strain rate sensitivity of 0.02, making the behaviour effectively rate insensitive.
The predicted strain distributions are shown in figure 13(a), alongside the HRDIC measurements. Although the predicted strain distribution is clearly very different from that measured, it has similar characteristics. The model is clearly unable to capture the slip band patterning and therefore the maximum value of strain predicted (∼0.8) is much less than that measured, which in some bands exceeds 2. There is however a relationship between the slip band density and the predicted strain intensity, that is, where the predicted strain is high, above and below the particle, the slip band density is higher. The direction of the dominant shear is predicted well, which suggests it is determined by the crystal orientation. Unlike the bands obtained experimentally, however, the bands of strain in the model are curved, which is a consequence of the plane strain boundary constraints imposed. The experimental strain map shows that the entire region is sheared and rotated during compression, which does not happen in the simulation. This rotation also causes the particle to rotate, which also does not happen in the model. Despite this, there are similarities in the way that the particle affects the deformation in the surrounding matrix, and the shape of the PDZ that develops. The change in slip activity is captured to some extent, with the positions of regions with low strain coinciding with those in the DIC measurements. From the rotation (both rigid-body and lattice) results, it can be seen that the direction of rotation predicted by CPFEM in the matrix around the particle generally matched with the results measured in DIC and EBSD, however the magnitudes of the rotations predicted are significantly larger than those measured.

There are two main reasons for the discrepancies between the modelling predictions and experimental results. The first lies in the unrealistic boundary conditions used. As discussed previously, the region studied shows a significant amount of shear indicating that the local deformation is less constrained than that imposed in the model. This added constraint can help explain the higher values of local misorientation predicted. This could also help explain why measurements on single crystals show larger rotations in the PDZ than those in polycrystals, since it is possible that in a polycrystal neighbouring grains can help relax the constraints locally. The second reason for the differences observed is the inability of the continuum CPFE model to simulate the slip pattern development in these materials. The model predicts a smooth, continuous variation in strain which is clearly not representative. In face of these limitations, it is perhaps surprising that such a simple model predicts many aspects of the local deformation well, suggesting it can be useful to understand effects of particle shape and grain orientation. However, it is clear that its inability to predict slip patterning makes it unable to predict the effect of particle size on the local rotation. This also explains why simple strain gradient plasticity theories where length scale considerations affect the work hardening but not the the distribution of strain are also unable to predict this effect [18].

5. Summary and conclusions
High resolution digital image correlation was used to map the deformation around different size particles in a polycrystalline Al-Si alloy during plane strain compression. These measurements revealed that in the material containing coarse particles deformation is inhomogeneous at the scale of the particle, forming a pattern of slip bands with a characteristic spacing. This pattern correlates well with the cell structure found in the material after deformation. The slip pattern is not crystallographically aligned, but its alignment depends on the crystal orientation. The presence of particles modifies the pattern locally, causing slip bands to intensify, broaden, bend and increase in number. These changes in the slip pattern, which can be interpreted as changes in local slip activity, cause the local lattice rotations usually observed in the particle deformation zone. However, when the particle size drops below the slip band spacing, so does the probability of particle slip band interaction. Since the strain between slip bands is significantly less than the strain in the slip bands, the deformation zone of a particle smaller than the slip band spacing is smaller and produces smaller rotations. The presence of very small, closely spaced particles
changes the deformation pattern everywhere, because slip cannot occur without interacting with
the particles. This has the effect of increasing the flow stress and of homogenising deformation.
Limited comparisons with crystal plasticity finite element modelling predictions show that these
models can capture important features of the PDZ like its shape and orientation, confirming
the idea that it depends on crystal orientation. However, because the model does not predict
the heterogeneous nature of deformation and its characteristic spacing it cannot predict the
effect of particle size on the development of the PDZ. One interesting implication is that in a
material containing both large particles and a distribution of closely spaced, fine particles, the
effect of size on the magnitude of the lattice rotation in the PDZ should disappear and show
good agreement with CPFE predictions.

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