



The Impact of Columnar and Equiaxed β -Grain Structures on Mechanical Anisotropy in High-Deposition-Rate Additively Manufactured $\alpha + \beta$ Titanium Alloys

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There is growing interest to produce $\alpha + \beta$ titanium alloys with high-deposition-rate additive manufacturing (DED-AM) processes for aerospace applications. However, there are still important aspects of their microstructure-mechanical property relationships that are not well understood, which are linked to the macro and microstructure heterogeneities generated by the AM processes and intrinsic titanium metallurgy that produce columnar β -grain structures. Trends in the literature, which are based primarily on Ti-6Al-4V data, have shown mechanical anisotropy is often present when samples exhibit coarse and columnar β -grain structures. This includes yield-stress and elongation anisotropy arising during uniaxial tensile testing, and crack growth rate anisotropy with high scatter recorded during fatigue testing, both of which are generally only tested in orientations parallel and perpendicular to the AM build direction. In this work, this mechanical anisotropy in $\alpha + \beta$ titanium alloys is investigated in more detail with Ti-6Al-4V and Ti-6Al-2Sn-4Zr-2Mo-0.1Si wire-arc additively manufactured test samples, comparing columnar parent β -grain structures to equiaxed grain structures. In particular, highlighting that the true yield-stress anisotropy in columnar grain samples is only revealed when testing the material at a 45 deg orientation away from the AM build direction. It is also shown that the large grain boundary α colonies that form on parent columnar β -grain boundaries have a significant impact on the fatigue crack growth rate data scatter. Refining the parent β -grain structures is demonstrated to resolve these issues and the related microstructure mechanisms were investigated in detail, using both experimental and crystal plasticity simulation methods. Finally, the formation and three dimensionality of the detrimental grain boundary α colonies that nucleate on columnar β -grain boundaries were investigated for the first time using in-situ SEM heating and 3D-EBSD techniques.

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I. INTRODUCTION

THE kilogram-per-hour deposition rates, build envelopes of several metres, and significant cost and energy savings that wire-based directed energy deposition additive manufacturing (DED-AM) technologies offer make such processes very attractive to the aerospace industry for building large near-net shape airframe components. However, achieving isotropic and reliable material properties is of importance to their wider scale adoption. Historically, titanium parts printed with DED-AM processes, like wire-arc AM (WAAM),^[1] have exhibited strongly textured, coarse and columnar β -grain structures, which lead to anisotropic mechanical properties and less predictable damage tolerance.^[2–6] However, recently, DED-AM technology has been advanced to the point where there are now several

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process modification options capable of producing large, titanium components with equiaxed and (near-)homogeneous grain structures with weak texture, especially for the most commonly used titanium alloy Ti-6Al-4V (Ti64).^[2,7-9]

The coarse and columnar β -grain structures in Ti64 that result from 'standard' DED-AM processing conditions exhibit grains growing upwards from the substrate, spanning many deposited layers, aligned close to the build-height/'normal' direction (ND).^[2,4,6] The formation of these problematic grain structures is mainly due to the lack of artificial grain refiners and low partitioning of the main alloying elements during solidification (e.g. partition coefficients for Al and V are $k_{Al} = k_V \approx 1$ ^[10-12]), preventing the development of sufficient constitutional undercooling necessary to nucleate new β grains in the moving melt pool.^[13] The β -phase body-centred-cubic (BCC) crystal structure has a $\langle 001 \rangle_\beta$ preferential growth direction and solidifies with the primary dendrite trunks orientated parallel to the largest thermal gradient, normal to the solidification front. Although the exact solidification texture that emerges will depend on the melt-pool shape and build strategy, over multiple layers the average preferential growth direction tends to be near-parallel to the layer normal direction (ND) that leads to the β grains developing a strong $\langle 001 \rangle_\beta \parallel$ ND fibre texture.^[2,3] This can lead to deposits containing coarse and columnar grains with only a small mutual misorientation around ND, which can sometimes be approximated to a single β crystal (e.g.^[14]).

In AM Ti deposits produced without grain refinement, this strong β texture leads to a pronounced α texture in $\alpha + \beta$ alloys like Ti64, which is determined by the $\{110\}_\beta \parallel \langle 0001 \rangle_\alpha, \langle 111 \rangle_\beta \parallel \langle 11\bar{2}0 \rangle_\alpha$ Burgers Orientation relationship (BOR) during the $\beta \rightarrow \alpha$ transformation.^[15] As there is no significant variant selection, the 12 possible α variants dilute the texture strength, but it can still affect the mechanical isotropy of components.^[3,16] This can be particularly problematic when combined with the coarse parent grain structure and local thermal history that can create undesirable room-temperature transformation microstructure and microtexture heterogeneity.^[17,18]

The columnar β -grain structures in DED-AM Ti64 can be refined by several approaches. Inter-pass deformation, where each deposited layer is rolled^[3,16,19] or machine-hammer peened^[20,21] between each layer, has been shown to be very successful in obtaining equiaxed β -grain structures, by promoting recrystallisation on reheating through the β transus, and is accompanied by a large reduction in texture strength. Another grain refinement technique that is often trialled is alloy modification. Additions like Fe, Co, Cu etc. ($k_{Fe} = 0.79$, $k_{Co} = 0.63$, $k_{Cu} = 0.39$ ^[10,11,22,23]) can be added to Ti64 to provide greater constitutional undercooling ahead of the solidification front and 'activate' nuclei in the melt pool resulting in more equiaxed microstructures with an accompanying texture reduction. However, alloy modification is seldom without cost. Alloying

additions—even in small amounts—will necessitate requalification, and can pollute recycling streams and produce unwanted second-phase particles that negatively impact mechanical properties (e.g.^[24]). Other refinement techniques include ultrasonic agitation of the melt pool to promote β -grain nucleation through liquid cavitation,^[25] but this is difficult to apply to full-scale industrial components. More recently it has also been demonstrated that melt-pool geometry can be manipulated by intelligent control of wire feed speed and heat source-travel speed. This has been proposed to encourage β -phase dendrites in the mushy zone to realign themselves with twin-type misorientations at steep inclination angles to the build direction, thereby creating new grains.^[9,26] In the long term, this may offer a more practical solution as it does not require any alloy modification or a secondary process step.

A summary plot of published DED-AM Ti64 yield stress (0.2 pct proof) data is provided in Figure 1, where values obtained from tensile-test samples orientated parallel (horizontal) and perpendicular (vertical) to the build-height direction are plotted against each other, with the $x = y$ line representing yield isotropy. It can be noted that all the data points are below this line, with a wide scatter, some significantly so. However, most points fall within a 10 pct difference demonstrating the trend for yield anisotropy produced by the $\alpha + \beta$ transformation microstructure, which is higher with samples tested in vertical orientations compared to those tested horizontally. In addition, although not discussed in detail in this paper, DED-AM Ti64 samples also exhibit even greater elongation anisotropy. This is shown in Figure 1(b) where the elongation to failure in the vertical test direction is generally higher than in the horizontal, and can commonly differ by as much as 50 pct. Also of note is the tendency for horizontal-direction elongation data to vary considerably. For example, in Reference 4 WAAM Ti64 repeated test samples exhibited a range of ± 129 pct of the average in the horizontal-direction elongation as compared to the ± 35 pct in the vertical direction.

It is further worth noting that an important limitation of the current tensile-test data available in the literature is the lack of uniaxial tensile testing of samples orientated at non-orthogonal directions to the AM build direction and, in particular, at 45 deg to it. This is an important consideration as, from a crystal plasticity point of view, the α transformation texture is inherited from the $\langle 001 \rangle_\beta \parallel$ ND fibre texture, which also often has a strong cube component. Therefore, by symmetry the least difference expected in the yield asymmetry would be between the orthogonal ND and WD directions, whereas an orientation 45 deg to these would be expected to give the largest difference. In addition, digital image correlation studies on small samples have shown that loading at 45 deg can promote premature failure due to shear localisation in the grain boundary α layer formed on some of the columnar β -grain boundaries.^[14]

Refining the columnar β -grain structures to produce an equiaxed- β microstructure in DED-AM Ti64 has

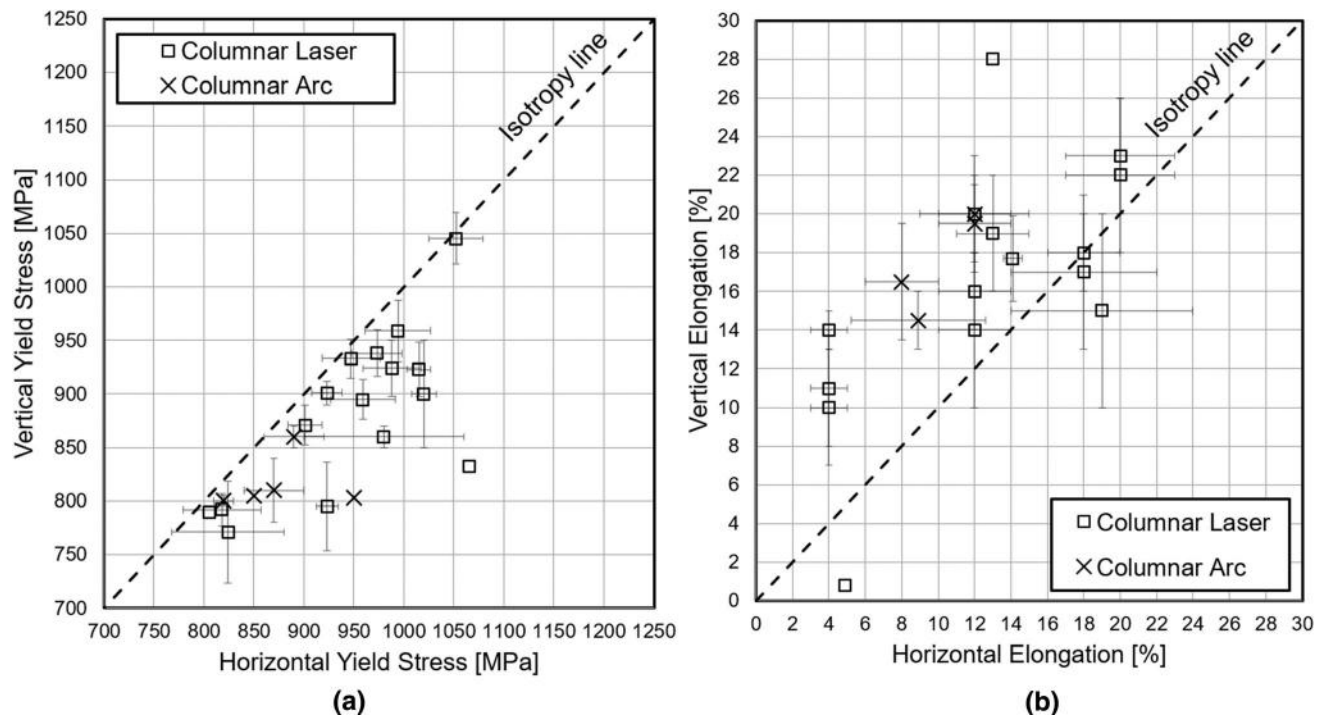


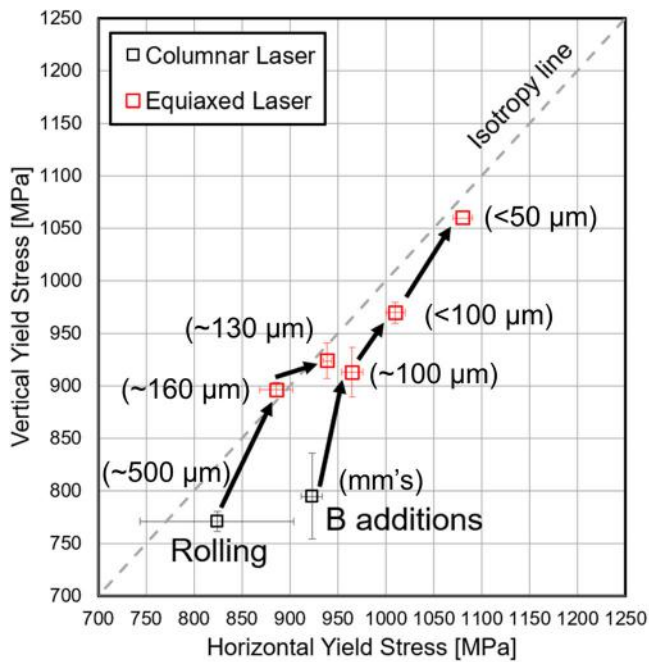
Fig. 1—Plots demonstrating the mechanical anisotropy of (a) yield stress and (b) elongation to failure in Ti64 DED-AM samples with columnar β -grain structures built using laser and plasma arc heat sources. Perfect isotropy is represented by the isotropy lines.^[4,6,16,19,20,24,27–29]

been shown to remove both yield-stress and elongation anisotropy. The number of reports is fewer for equiaxed structures than for columnar, but the limited data available in the literature has been summarised in Figure 2 and Table I. The summary table also includes data for Ti6242—an alloy designed for higher temperature application—for comparison to Ti64, though there is very little data for this alloy in the literature, so only a WAAM Ti6242 dataset by the current authors is included, along with an example of a powder-bed-fusion process from the literature. The plots in Figure 2 show the elimination of anisotropy with β -grain size reduction, for inter-pass deformation^[16,19,20] and alloy modification.^[24] It can be noted that the reduction in parent β grain-size also coincides with an increase in yield strength produced by the room-temperature $\alpha + \beta$ transformation microstructure. For example, Martina *et al.*^[16] have demonstrated that inter-pass rolling can increase the yield strength of WAAM Ti64 samples by 150 and 180 MPa in the horizontal and vertical directions, respectively. This strengthening effect has yet to be sufficiently explained, as the yield stress is dominated by the microstructure and texture of the α phase and not the parent β -grain size when it is still relatively coarse ($> 200 \mu\text{m}$), compared to the α lath size.^[15]

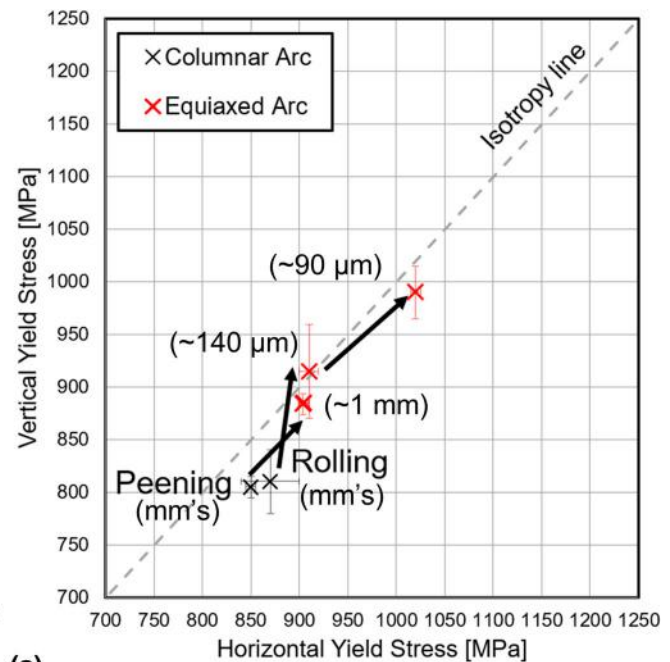
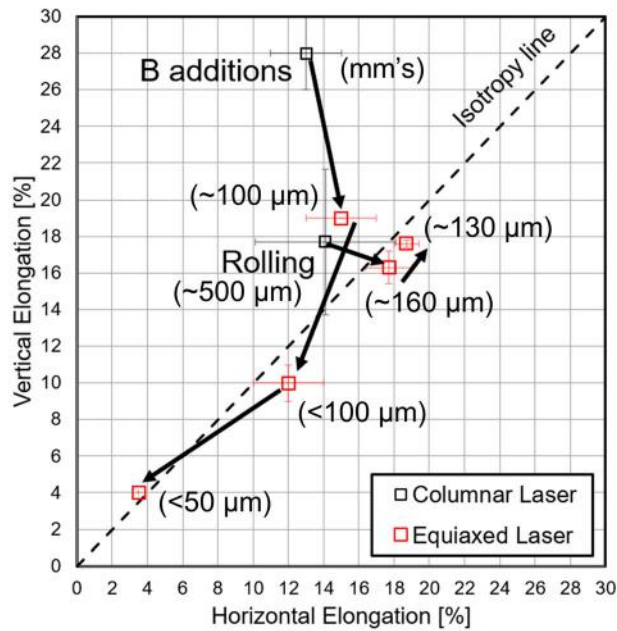
The coarse microstructure and microtexture related to columnar β -grain structures can also contribute to anisotropy in fatigue crack propagation rates in DED-AM Ti64 samples, which is an important consideration for aerospace applications. However, due to the test duration and large sample sizes, fatigue tests that allow examination of crack growth behaviour of

DED-AM Ti64 parts tend to be conducted in small batches, and there is currently insufficient data to evaluate the statistical scatter. In addition, the machined notch used to guide crack initiation is generally placed within a sample without any regard for the local macro/microstructure variation. Since heterogeneities in DED-AM Ti64 samples, such as columnar grain boundaries and heat affected zone bands (HAZ) bands, are often millimetres apart (*e.g.* Figure 3), the impact these features have can be significant. For example, in a recent study with WAAM Ti64,^[5] it was demonstrated that fatigue crack growth rates are generally higher in the horizontal (WD) direction than in the vertical. This difference was more significant in the $\Delta K < 25 \text{ MPa m}^{1/2}$ regime, where the microstructure influence on crack growth behaviour dominates, but large scatter was also observed between tests. This anisotropy and scatter were attributed to the variance in crack tortuosity encountered in the different growth directions, due to microtexture heterogeneity and microstructure features, such as HAZ bands and grain boundary α colonies.

Because of the importance of achieving isotropy and less scatter in the mechanical performance of large-scale titanium AM components, the purpose of this study is to probe in greater depth the mechanisms that control yield anisotropy in wire-based DED-AM Ti components and how β -grain refinement alters the mechanical properties overall. This has been achieved by examining more closely the impact of the β -phase grain structure and texture on the $\alpha + \beta$ transformation microstructure and texture, and its influence on plasticity. Using two



(a)



(b)

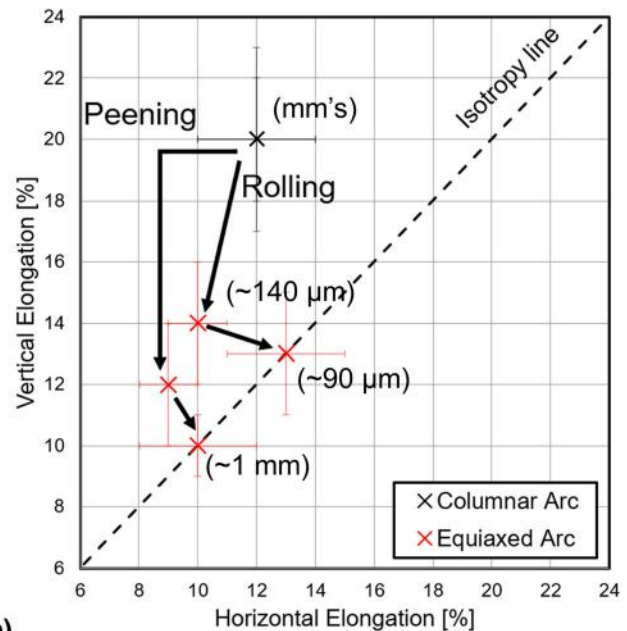


Fig. 2—The reduction of mechanical anisotropy in the (a) yield stress and (b) elongation to failure by refining the columnar β -grain structures to equiaxed in Ti64 DED-AM samples with columnar β -grain structures built using laser and plasma arc heat sources. Perfect isotropy is represented by the dashed lines, and progressive reduction of β -grain sizes are represented by the arrows (grain sizes given in brackets). Refinement techniques used were inter-pass deformation with (machine hammer) peening^[20] and rolling (with decreasing peening pitch and increasing layer height reductions, respectively),^[16,19] and alloy modification to Ti64 using boron (B) additions up to 1 wt pct.^[24]

example alloys—Ti64 and Ti6242—the following key questions will be considered:

- What is the extent and cause of yield-stress anisotropy in columnar grain samples?
- What is the impact of these structures on damage tolerance?

- How do columnar parent β -grain structures influence the room-temperature transformation microstructure to produce the above negative effects?
- And how does β -grain refinement remove yield-stress anisotropy and produce a yield-stress increase?

Table I. Summary of the Tensile Properties of Ti64 and Ti6242 Produced by Various DED-AM Processes Using Laser, Electron Beam, and Plasma Arc Heat Sources, Where σ_{YS} = Yield Stress, ε = Elongation to Failure, Horizontal = Heat Source Travel/Welding (WD) or Transverse (TD) Directions, and Vertical = Build-Height 'Normal' Direction (ND)

Process	σ_{YS} Horizontal [MPa]	σ_{YS} Vertical [MPa]	ε Horizontal [Pct]	ε Vertical [Pct]	Rolling reduction [Pct]	Peening pitch [mm]	B Alloy Additions [Wt Pct]	Grain Structure/size	References
Ti-6Al-4V Laser	959 $\pm$ 32	895 $\pm$ 19	18 $\pm$ 2	18 $\pm$ 2				columnar/mm's	6
	947 $\pm$ 29	933 $\pm$ 18	18 $\pm$ 4	17 $\pm$ 4					
	1015 $\pm$ 12	923 $\pm$ 25	12 $\pm$ 3	20 $\pm$ 3					
	988 $\pm$ 29	924 $\pm$ 26	20 $\pm$ 3	22 $\pm$ 4					
	923 $\pm$ 15	901 $\pm$ 11	19 $\pm$ 5	15 $\pm$ 5					
	901 $\pm$ 17	871 $\pm$ 19	13 $\pm$ 2	19 $\pm$ 3					
	994 $\pm$ 33	959 $\pm$ 29	12 $\pm$ 2	14 $\pm$ 4					
	973 $\pm$ 25	938 $\pm$ 22	20 $\pm$ 3	23 $\pm$ 3					
	818 $\pm$ 39	792 $\pm$ 15	4 $\pm$ 1	11 $\pm$ 3					27
	980 $\pm$ 80	860 $\pm$ 10	4 $\pm$ 1	10 $\pm$ 3					28
	805	790	12 $\pm$ 2	16 $\pm$ 2					29
	1020 $\pm$ 12	900 $\pm$ 50	4 $\pm$ 1	14 $\pm$ 1					30
	1065	832	5	1					31
	923 $\pm$ 11	795 $\pm$ 41	13	28					24
Laser + Boron Additions	965 $\pm$ 11	913 $\pm$ 24	15 $\pm$ 2	19 $\pm$ 0				columnar/mm's	
	1010 $\pm$ 10	970 $\pm$ 10	12 $\pm$ 1	10 $\pm$ 1				columnar/mm's	
	1080 $\pm$ 10	1060 $\pm$ 0	4 $\pm$ 0	4 $\pm$ 0				columnar/mm's	
	824 $\pm$ 56	771 $\pm$ 48	14 $\pm$ 1	18 $\pm$ 2				partially columnar/ $\sim$ 100 μ m	
Laser + Hot Rolling	886 $\pm$ 17	896 $\pm$ 7	18 $\pm$ 1	16 $\pm$ 1				equiaxed/ $<$ 100 μ m	
	939 $\pm$ 4	924 $\pm$ 17	19 $\pm$ 1	17 $\pm$ 0				equiaxed/ $<$ 50 μ m	
Plasma Arc	890 $\pm$ 30	860 $\pm$ 10	8 $\pm$ 2	17 $\pm$ 3	0			partially columnar/ $\sim$ 500 μ m	19
	950	803	9 $\pm$ 2	15 $\pm$ 2	37.5			equiaxed/ $\sim$ 160 μ m	
Plasma Arc + Cold Rolling	870 $\pm$ 30	810 $\pm$ 30	12 $\pm$ 2	20 $\pm$ 2	50			equiaxed/ $\sim$ 130 μ m	
	910 $\pm$ 10	915 $\pm$ 45	10 $\pm$ 1	14 $\pm$ 2				columnar/mm's	27
Plasma Arc + Cold peening	1020 $\pm$ 5	990 $\pm$ 25	13 $\pm$ 2	13 $\pm$ 2				columnar/mm's	4
	850 $\pm$ 5	805 $\pm$ 10	12 $\pm$ 1	20 $\pm$ 3	0			Equiaxed/ $\sim$ 140 μ m	16
Ti-6Al-2Sn-4Zr-2Mo-0.1Si	905 $\pm$ 5	885 $\pm$ 2	9 $\pm$ 1	12 $\pm$ 2	18			Equiaxed/ $\sim$ 90 μ m	
	904 $\pm$ 5	885 $\pm$ 10	10 $\pm$ 2	10 $\pm$ 1				columnar/mm's	20
Plasma Arc + Cold Peening Electron Beam (PBF)						0		equiaxed/ $\sim$ 1 mm	
						4.0		equiaxed/ $\sim$ 1 mm	
						0.5		equiaxed/ $\sim$ 1 mm	
								columnar/mm's	32 and this work.
								equiaxed/ $\sim$ 260 μ m	
								columnar/mm's	33

All β -grain structures were columnar unless the following refinement mechanisms were used: alloy modification using boron additions, or inter-pass deformation using hot/cold rolling or cold machine-hammer peening

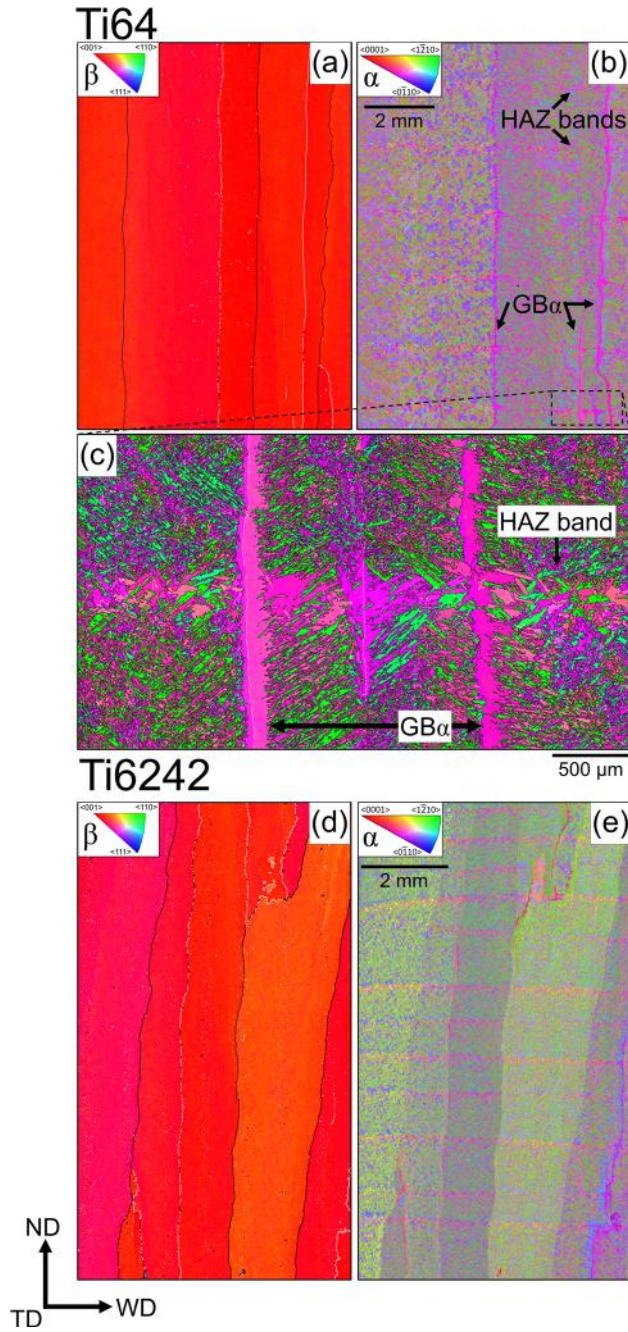


Fig. 3—(a, d) Reconstructed- β and (b, e) α -phase EBSD maps of the example WAAM Ti64 and Ti6242 columnar grained samples showing the highly textured parent β -grain structures, HAZ bands, and grain boundary α (GB α) transformation microstructure heterogeneities. (c) A magnified region of the α phase map in (b) showing the HAZ bands and GB α in more detail.

II. EXPERIMENTAL AND MODELLING METHODS

A. Material Deposition

All material used in this paper was sourced from multiple independent studies that all used the WAAM process with commercial Ti64 and Ti6242 standard wire feedstock. For brevity, only fabrication parameters

considered relevant are detailed in Table II, but the reader is invited to follow references therein for more details. All samples were fabricated using wire feedstock with 1.2 mm diameters and deposited under a protective argon atmosphere to avoid oxidation. Samples that were built to compare columnar and equiaxed β -grain structures were deposited with a controlled inter-pass temperature, where the substrate was left to cool to a certain temperature before the next layer was deposited. This was to ensure that differences in mechanical behaviour could be attributed to the parent β -grain structure and not differences in the thermal history that affect the transformation microstructure. The WAAM reference frame used throughout is defined as: normal or build-height direction $\equiv$ ND, welding or heat-source travel direction $\equiv$ WD, and transverse direction $\equiv$ TD.

B. Mechanical Testing

Ti64 dog-bone tensile-test specimens of 4 mm thickness, 6 mm width, and 30 mm gauge length were extracted from the WAAM walls (following the BS EN 2002-1:2005 standard^[35]), orientated in both WD and ND directions, from machine-hammer peened and as-deposited samples. Tensile testing was carried out with a grip velocity of 2 mm/min, and four samples were tested in each orientation with 0.2 pct proof stress, ultimate tensile stress, and elongation to failure data averaged and reported with a 1 standard deviation error measurement. All tests were carried out on an electromechanical Instron test machine with a 100 kN load cell at room temperature, measuring strain using digital image correlation from an applied metal-paint speckle pattern.

For the Ti6242 tensile testing, flat dog-bone specimens of 5 mm thickness, 6 mm width, and a 32 mm gauge length were extracted from the WAAM walls (following the ASTM E8 standard^[36]), orientated in the WD and ND directions. Tensile testing was carried out with a grip velocity of 2 mm/min. Only two samples were tested in each condition/orientation, so averages were calculated with no error applied. All tensile tests were carried out on an Instron electromechanical test machine with a 100 kN load cell at room temperature, measuring strain with a non-contact laser video extensometer.

For both Ti64 and Ti6242 crack growth rate tests, notched compact tension specimens following the ASTM E647 standard^[37] were extracted from the test walls with their crack planes orientated parallel to ND and WD. Increasing stress intensity factor range (ΔK) crack growth rate tests were then conducted until the samples failed, using a constant loading amplitude with a standard sinusoidal waveform and a cyclic load ratio of $R = 0.1$. The crack growth was measured by a travelling optical microscope so change in crack length relative to the number of cycles (da/dN) could be plotted against ΔK . Additional tests were conducted that were stopped before failure could occur, so that the crack propagation in relation to the microstructure could be studied in more detail.

Table II. A Summary of the WAAM Sample Deposition Parameters—for More Details, See References Provided

Alloy Grain Structure	Deposition Strategy Grain-Refinement Measures	Inter-Pass Temperature [°C]	Wire Feed Speed [mm/s]	Travel Speed [mm/s]	Figures	References
Ti64 Columnar and Equiaxed	oscillation none and machine-hammer peened	140	50	6.2	3(a) through (c), 4(a) and (c), 5	5, 20
Ti64 Columnar and Equiaxed	single bead none and machine-hammer peened	140	40	5	6(a) through (d), 7(a), 8, 9(a), 11(a) and (b), 12, 15, 16	20
Ti64 Columnar and Equiaxed	single bead none	not controlled	40	6	13, 14	34
Ti6242 Columnar and Equiaxed	single bead machine-hammer peened	60	33.3	5	3(d), (e), 4(b), (d), (f), (h), 6(e), (f), 7(b), 10, 11(c, d)	21, 32

Schematics for all mechanical test specimens have not been included for brevity—please see the references listed in Table II.

C. Microstructure Characterisation

All samples for microstructure characterisation were metallographically prepared using silicon carbide papers with progressively increasing grit, then polished directly with a solution of water, OPS, and hydrogen peroxide with a ratio of 6:1:1. All samples were cleaned thoroughly with soapy water before examination.

Sample microstructures were characterised primarily by electron backscatter diffraction (EBSD) using a *Thermo Fisher Apreo* field emission gun scanning electron microscope (FEG-SEM) equipped with an *Oxford Instruments' Symmetry 2* EBSD detector using *AZtec* acquisition software. EBSD maps were collected using a SEM accelerating voltage of 20 kV, probe currents between 30 and 100 nA, sample tilt of 70 deg, with step sizes optimised to the microstructure features characterised. All maps and texture data were processed using *Oxford Instruments' AZtecCrystal*. EBSD maps are presented in inverse pole figure colouring with the orientation reference parallel to ND, and texture data is plotted as contoured pole figures scaled in multiples of random density (MRD). Parent β -grain structures were reconstructed from the acquired α -phase data using the *AZtecCrystal Parent Grain Analysis* tool, where the minimum deviation for child grain detection was 5 deg.

Microstructures were further characterised using backscatter electron (BSE) imaging. This was conducted on an *FEI Magellan* FEG-SEM equipped with a 4-quadrant BSE detector. For single images, a 5 kV accelerating voltage, a 1.6 nA probe current, and a 4 mm working distance was used. Inter-lamellar spacings of α laths were measured using a bespoke MATLAB software—more details can be found in Reference 38. For multi-image scans to investigate α lath major axis length orientation relative to ND, large areas of the microstructure were surveyed using the *FEI MAPS* software to collect $30 \times 30 \mu\text{m}$ tiles across 3 lines 10 mm in length. To prioritise collection speed over the signal to noise ratio, the probe current was increased to 6 nA so a shorter image dwell time could be used. The images were then processed using a bespoke *Python* code that segments the images into individual grains, to measure each lath's orientation relative to the image y -axis. Each image was inverted, to treat the retained β as background, and then white balanced with a percentile clip of 40 pct to normalise the brightness of the α laths. *Niblack* thresholding, with a window size of 29 pixels, was then applied to binarise the images, along with area closing with a threshold of 1000 pixels to remove any noise within each lath. An erosion was then applied to the binary image, with nine erosions, to separate any overlapping grains, and a distance transform applied to identify grain centres for labelling. A watershed algorithm was used to fill from the grain centres, applied on the original binary image (before erosion) to provide the individual grain segmentations. Once the grains were segmented, each grain was treated

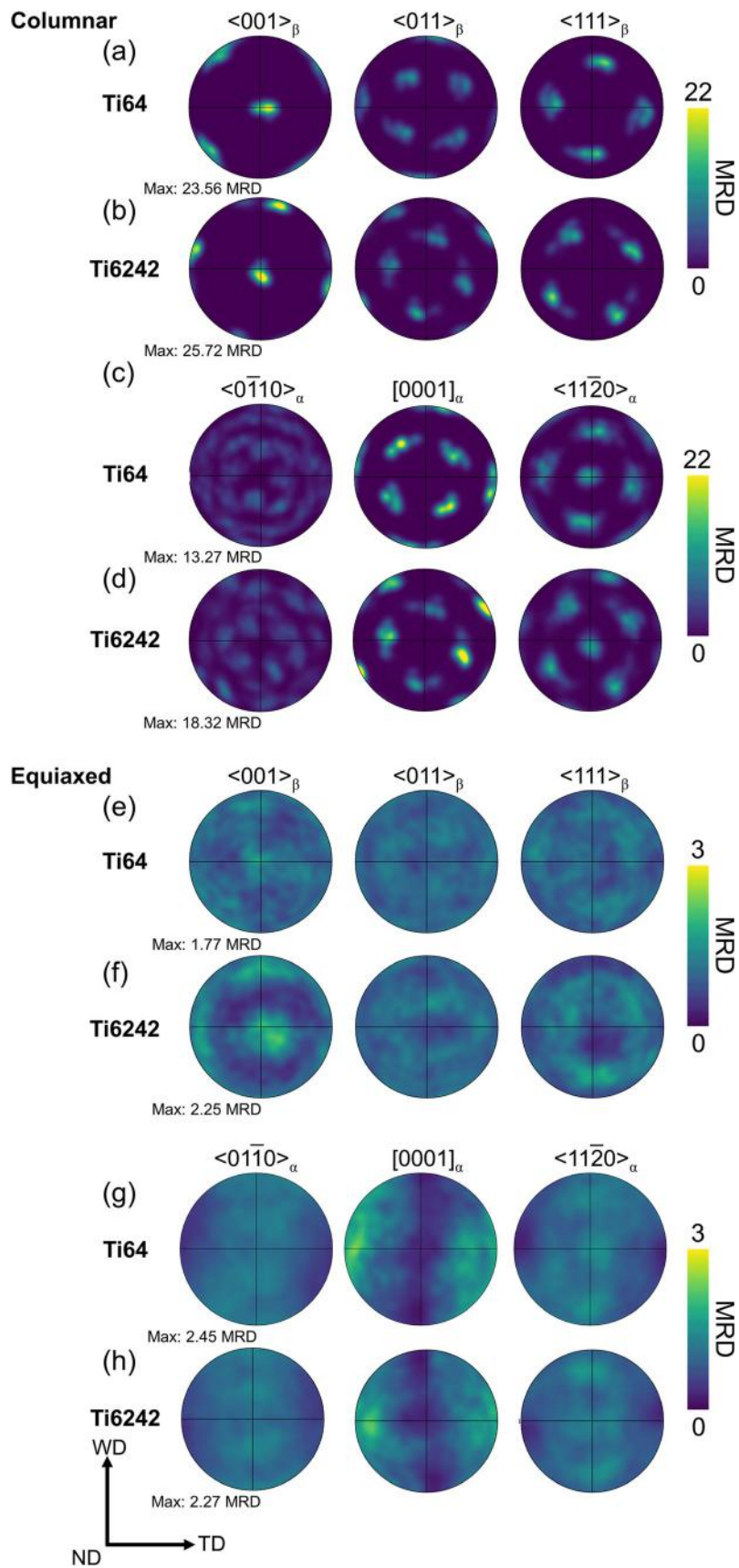


Fig. 4—Pole figures showing the texture of Ti64 and Ti6242 WAAM for (a–d) columnar grained samples (Fig. 3) and (e–h) equiaxed grained samples (Fig. 7). Please note the change of MRD scales.

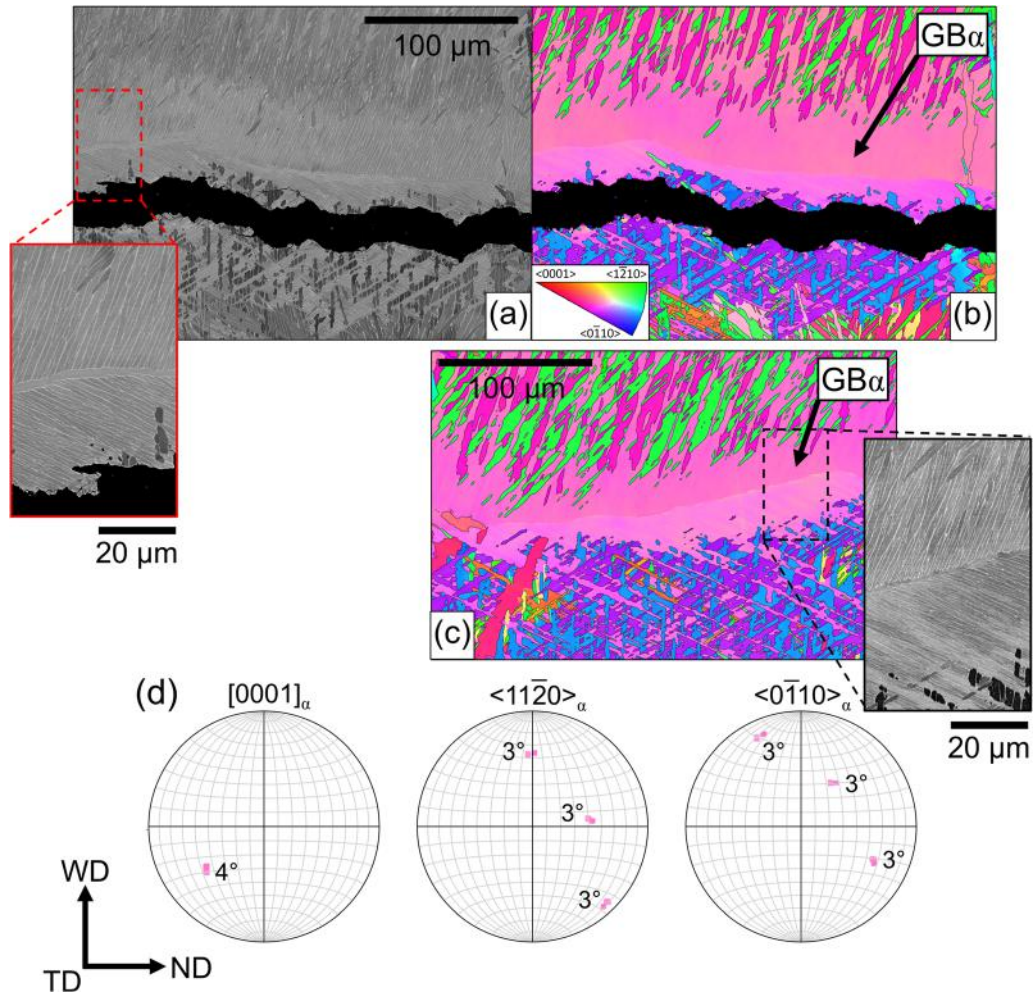


Fig. 5—Examples of grain boundary α (GB α) in the cracked example Ti64 WAAM sample [Fig. 12(b)]: (a, b) direct comparison of its appearance in (a) backscatter electron imaging and (b) EBSD, (c) magnified regions of interest, (d) pole figures showing the orientations of the GB α either side of the parent β -grain boundary.

as an individual image. The covariance matrix for each grain was calculated and the principal eigenvector of the covariance matrix then gives the grain orientation, as a vector. This was then converted into an angle relative to the y -axis (bottom edge) of each image. This code can be found at Reference 39.

To study the Ti64 $\beta \rightarrow \alpha$ phase transformation in real time, a *Gatan* in-situ Murano SEM heating stage was used in conjunction with EBSD mapping on an *FEI Nova* FEG-SEM with an Oxford Instruments' Nordlys Max² detector equipped with an alumina coated phosphor screen to block out IR radiation. $2 \times 1 \times 1$ mm samples were prepared as documented above and adhered to silicon chips using carbon paste. A high-purity zirconium block was also added to the chip as an 'oxygen getter' to preferentially bond with remnant oxygen in the SEM chamber. The SEM chamber was additionally left to pump overnight to obtain the best vacuum possible for the experiments. The heating stage temperature was monitored indirectly by a thermocouple in contact with the heating chip, and is found to have an error of ± 20 °C. The sample was first heated to

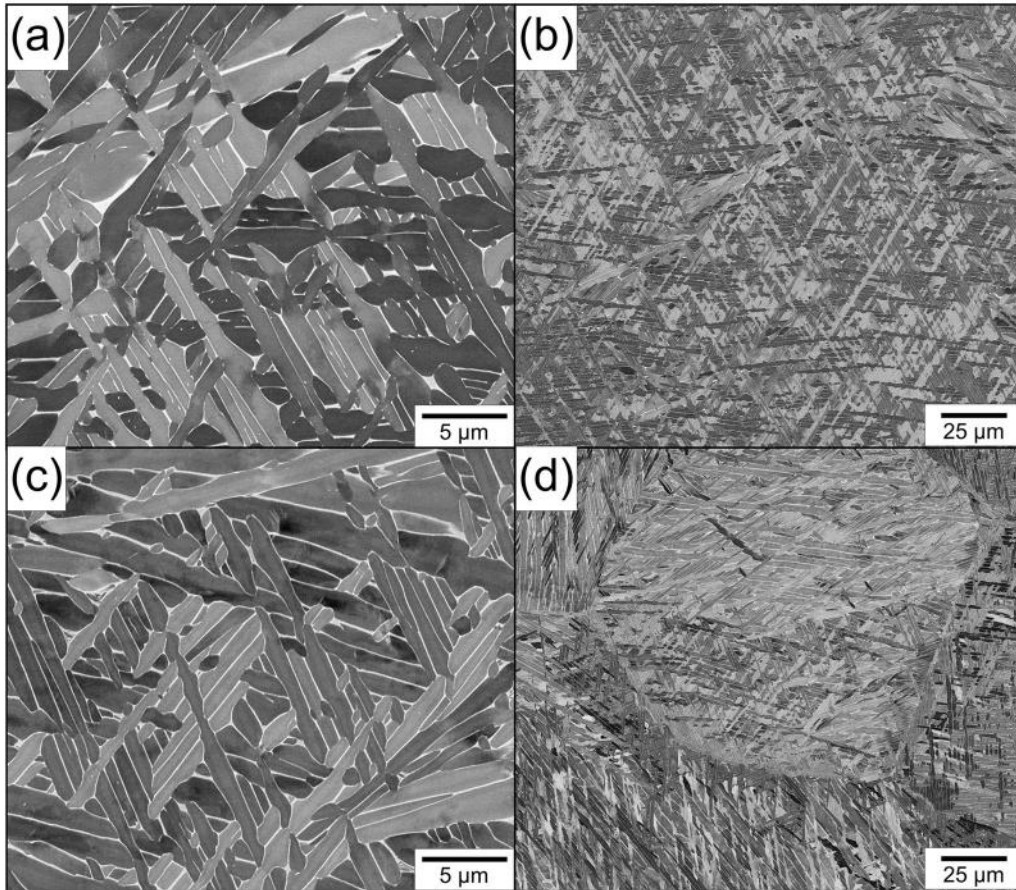
1000 °C into the 100 pct β -phase regime, where the initial β -grain structure was mapped with EBSD; the sample was then cooled and held for further EBSD mapping at 900 and 750 °C, with a cooling rate of ~ 0.3 °C/s. The microstructure was allowed to stabilise for several minutes at each temperature hold before mapping was started. For more details on the in-situ SEM heating technique, please see Reference 40.

The 3D EBSD scan was conducted on a *Thermo Scientific Helios 5* FEG-SEM equipped with a Xe^+ plasma focussed ion beam (PFIB), a femto-second laser, and an *Oxford Instruments' Symmetry* EBSD detector (for more details, see^[41]). A matchstick sample was first extracted from the Ti64 WAAM wall, polished on its top face, then adhered to an SEM stub with its bulk overhanging. After the area of interest was identified on the polished face with (2D) EBSD, the femto-second laser was used to cut away excess material until a block of $\sim 300 \times 300 \times 300$ μm protruded from the sample bulk. The perpendicular face was then serially EBSD mapped and sliced using the PFIB. For this, the sample was mounted on a pre-tilted holder so that the

examination surface could be moved between positions perpendicular to the ion beam for PFIB slicing and 70 deg to the electron beam for EBSD mapping, with just a 180 deg stage rotation and a constant stage tilt of 16 deg (schematic diagrams can be found in Reference 42).

PFIB slicing was carried out with a 30 kV accelerating voltage and a 0.5 nA probe current, removing 0.2 μm of material per slice, using fiducial tracking to maintain accurate stage positions for the slicing and a rocking mill at ± 5 deg to limit topography from PFIB-induced

Ti64



Ti6242

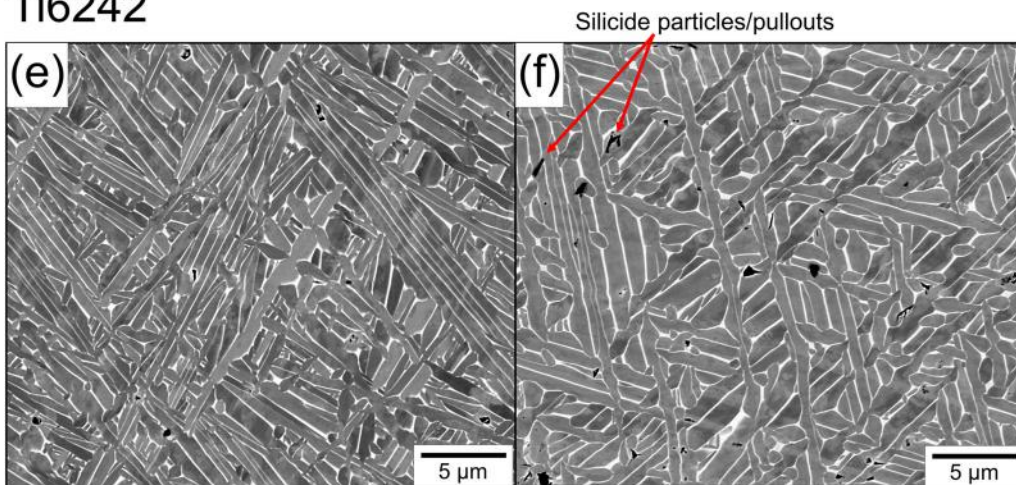


Fig. 6—Typical WAAM basketweave microstructures at different magnifications for (a, b) as-deposited Ti64, (c, d) machine hammer peened Ti64, (e) as-deposited Ti6242,^[21] and (f) machine hammer peened Ti6242. Note: the labelled silicides particles/pullouts in the Ti6242 microstructures have been identified by SEM-EDS previously^[21].

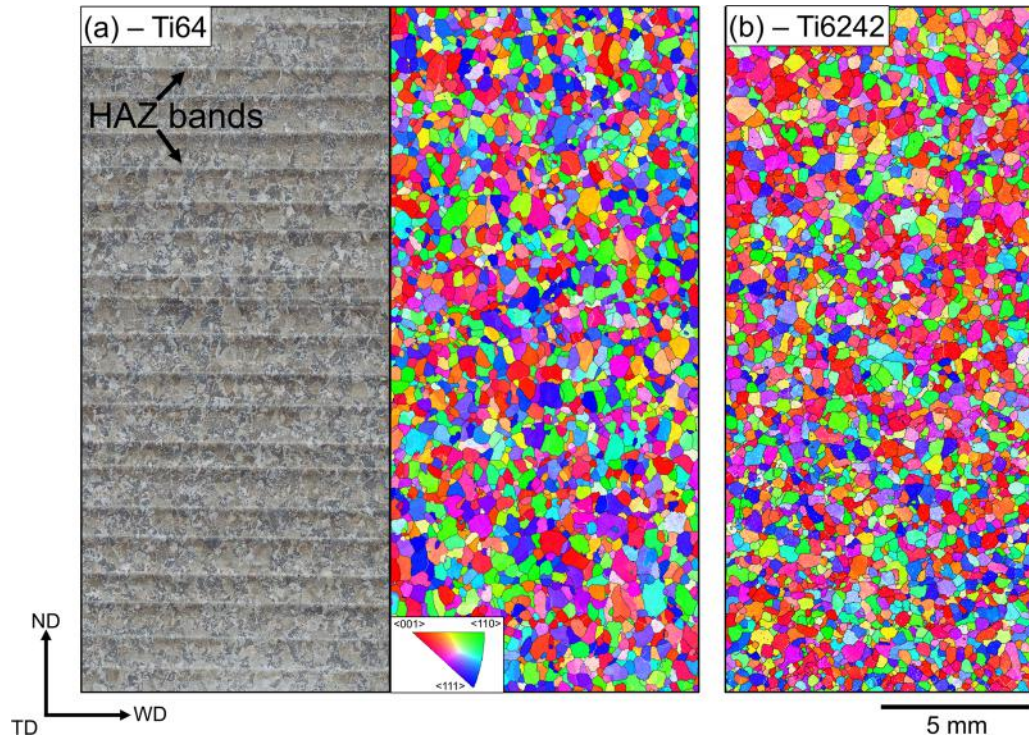


Fig. 7—(a) Optical macrograph and reconstructed- β EBSD map of the peened Ti64 WAAM sample and (b) reconstructed- β EBSD map of the peened Ti6242 WAAM sample. The reconstructed- β and α textures are displayed in the pole figures in Figs. 4(e) through (h), respectively.

curtains.^[43] EBSD maps were collected every second slice (*i.e.* every $0.4\ \mu\text{m}$) with an accelerating voltage of 20 kV and a step size of $0.4\ \mu\text{m}$ was used, resulting in a voxel size of $0.4 \times 0.4 \times 0.4\ \mu\text{m}$. Reconstruction of the 3D EBSD was facilitated by *Dream.3D v.6.5.163*^[44] software and imaged in *Paraview*.^[45]

D. Crystal Plasticity Simulations

Crystal plasticity (CP) deformation simulations were used to investigate the plasticity behaviour in Ti64 WAAM materials, using both synthetic and pseudo-3D microstructures from experimental 2D EBSD datasets. For all simulations, only the α phase was included as there is < 10 pct volume fraction β phase in Ti64 and its contribution to deformation behaviour was assumed to be insignificant for this study. CP simulations require elasticity and plasticity data input to function for a particular material system to produce statistically reliable replication of deformation behaviour. Critically resolved shear stresses (CRSSs) for α -phase basal ($\{0001\}\langle 11\bar{2}0 \rangle$), prismatic ($\{01\bar{1}0\}\langle 11\bar{2}0 \rangle$), and 2nd order pyramidal ($\{11\bar{2}2\}\langle 11\bar{2}3 \rangle$) slip systems were determined by calibration in visco-plastic self-consistent (VPSC) simulation tensile loading (for brevity)^[46] to known yield stresses in the ND and WD orientations (* in Table IV). 100 crystal (Euler) orientations were randomly extracted from the corresponding material texture and used as simulation input to replicate the anisotropic tensile behaviour.

Simulation was then moved to the CP simulation package DAMASK^[47] that replicates deformation in polycrystal microstructures with spatially resolved grain orientations, so that features that are statistically more likely to lead to stress/strain concentration could be identified. A finite strain elasto-visco-plastic model is implemented in DAMASK and a fast Fourier transform (FFT) based method is used to solve for mechanical equilibrium, which allows efficient simulation of cuboidal volumes with simple imposed deformation. A power-law flow with Voce-type hardening was used, which is similar to the constitutive behaviour in the VPSC model. To complete calibration of the simulation parameters, a synthetic 3D microstructure consisting of 100 grains, generated by Voronoi tessellation, was used to determine the strain hardening parameters that would match the lack of any significant hardening seen in experimental (engineering) stress-strain curves (*e.g.* Figure 9). All input parameters for the CP simulations are listed in Table III. Tensile-test simulations of interest were then carried out using the same elasticity and plasticity parameters, loaded in orientations parallel to WD, ND, and 45 deg to ND (around TD), but with either the synthetic 3D microstructure or pseudo-3D microstructures augmented from direct EBSD map input.

2D α -phase EBSD maps for simulation input were restricted to 1000×1000 pixels to ensure simulations could be completed with practical computational resources. To capture the fine WAAM Ti64 lamellar microstructure, EBSD maps were collected with a step size of $< 1\ \mu\text{m}$, providing sufficient resolution to capture

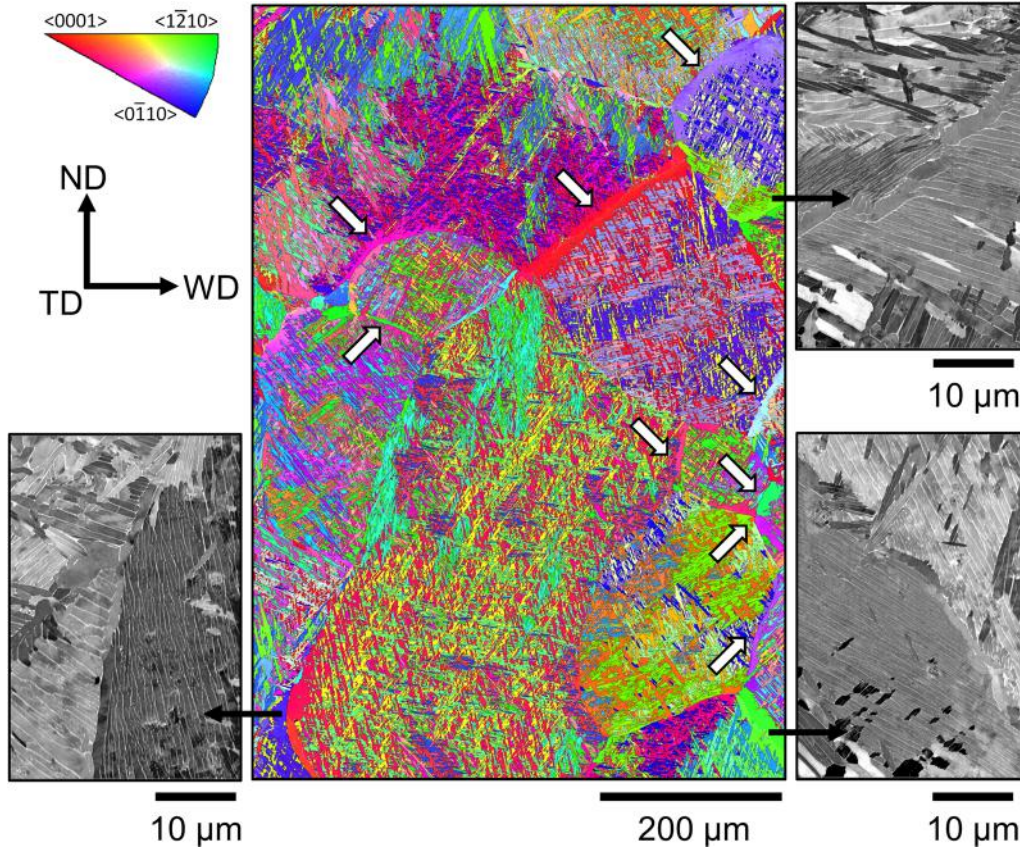


Fig. 8—Example α EBSD maps (centre) highlighting grain boundary α layers seen in the peened Ti64 WAAM sample with magnified backscatter electron insets showing their features in more detail.

‘grain’-to-‘grain’ interaction over a statistically large area. The EBSD maps were then extruded by 4 pixels to generate a pseudo 3D volume. As the simulation applies periodic boundary conditions, a buffer region of low-tensile material was included on the ‘EBSD’ surface to create the condition of a free surface.^[48] Tensile loading was applied only in the plane of the original 2D EBSD map. Data input, simulation, and results processing (simulated stress-strain curves) were facilitated by the MatFlow package developed by A. Plowman *et al.*^[49] Simulations were performed using the computation shared facility cluster hosted by the University of Manchester, using a single node and up to 16 cores and 300 GB of memory.

III. RESULTS

A. Typical Microstructures and Textures

1. Conventional deposits with coarse and columnar β -grain structures

Examples of conventional as-deposited WAAM samples sectioned in the ND-WD cross section are shown in Figure 3. The typical coarse and columnar grain structures and microtextures found for the two alloys, Ti64 and Ti6242, can be seen in the reconstructed β -phase EBSD maps in Figures 3(a) and (d),

respectively. The columnar grains span many deposited layers, reach centimetres in length, and are separated by vertical grain boundaries (GBs) that are approximately parallel to ND in this section plane. The β -phase textures present in the EBSD maps in Figures 3(a) and (d) are depicted in the β -phase pole figures in Figures 4(a) and (b) and clearly show common $\langle 001 \rangle_\beta \parallel \text{ND}$ textures, with strong alignment of the $\langle 001 \rangle_\beta$ crystal directions in ND with partial fibres created by slight rotation about this axis. Due to the poor grain sampling statistics in these maps, without analysing multiple cross sections, it is unclear if overall these wall samples contain *full* fibre textures or have strong cube components with $\langle 001 \rangle_\beta$ directions aligned parallel to both WD and TD.

The microstructure and texture of the room-temperature α phase that formed from the parent β grains in Figures 3(a) and (d) are shown in Figures 3(b) and (e), in both low magnification—covering multiple columnar β grains—and in high magnification for Ti64 in Figure 3(c), to capture more detail of the commonly termed ‘basketweave’ microstructure. The α laths in both alloys adopt crystallographic orientations from the 12 variants available determined by the BOR, and so the strong $\langle 001 \rangle_\beta \parallel \text{ND}$ texture inherited from the β phase is diluted by the large number of possible α variants (*i.e.* without significant variant selection). This is shown in

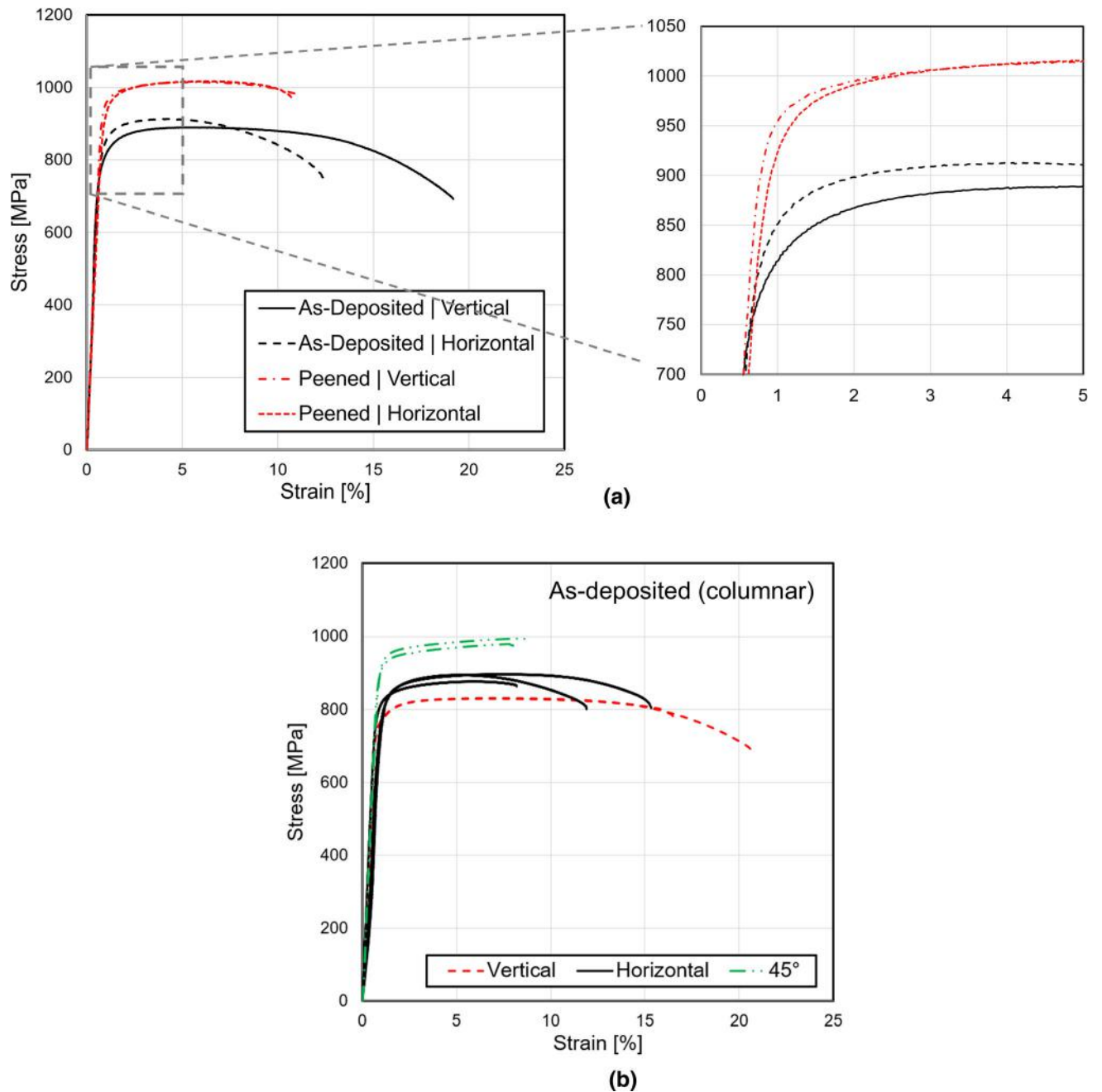


Fig. 9—(a) Comparison of typical tensile engineering stress-strain curves for the Ti64 WAAM samples tested in horizontal and vertical directions (parallel to WD and ND) for as-deposited columnar and peened equiaxed grain samples, and (b) comparison of as-deposited tensile tests with samples loaded in horizontal and vertical directions, and at an orientation 45 deg to the build-height direction.

the pole figures in Figures 4(c) and (d) where the $\langle 001 \rangle_{\beta}$ || ND β texture can be seen to translate into a partial fibre α transformation texture with a uniform distribution across the possible α variants, whereby the poles in the $[0001]_{\alpha}$ pole figure are rotated slightly about ND with a ~ 45 deg precession. That is, the basal planes are preferentially aligned ~ 45 deg to ND, WD, and TD through the alignment with the 6 $\{011\}_{\beta}$ habit planes, reflecting the cubic symmetry of the β phase. This fibre texture is more obvious in the Ti64 pole figures due to

the slightly greater spread in the β fibre texture about ND [Figure 4(a)].

Although all 12 α variants are uniformly present in the bulk textures, within each prior β grain they are not distributed homogeneously throughout the microstructure. Instead, diffuse microtexture colonies commonly consisting of (usually) 3 specific α variants (tri-variant colonies) repeat in an irregular pattern across each grain, as can be seen in α -phase EBSD maps for both alloys due to the distinct IPF colouring of the colonies [e.g. Figures 3(b) and (e)]. Importantly, due to the BOR

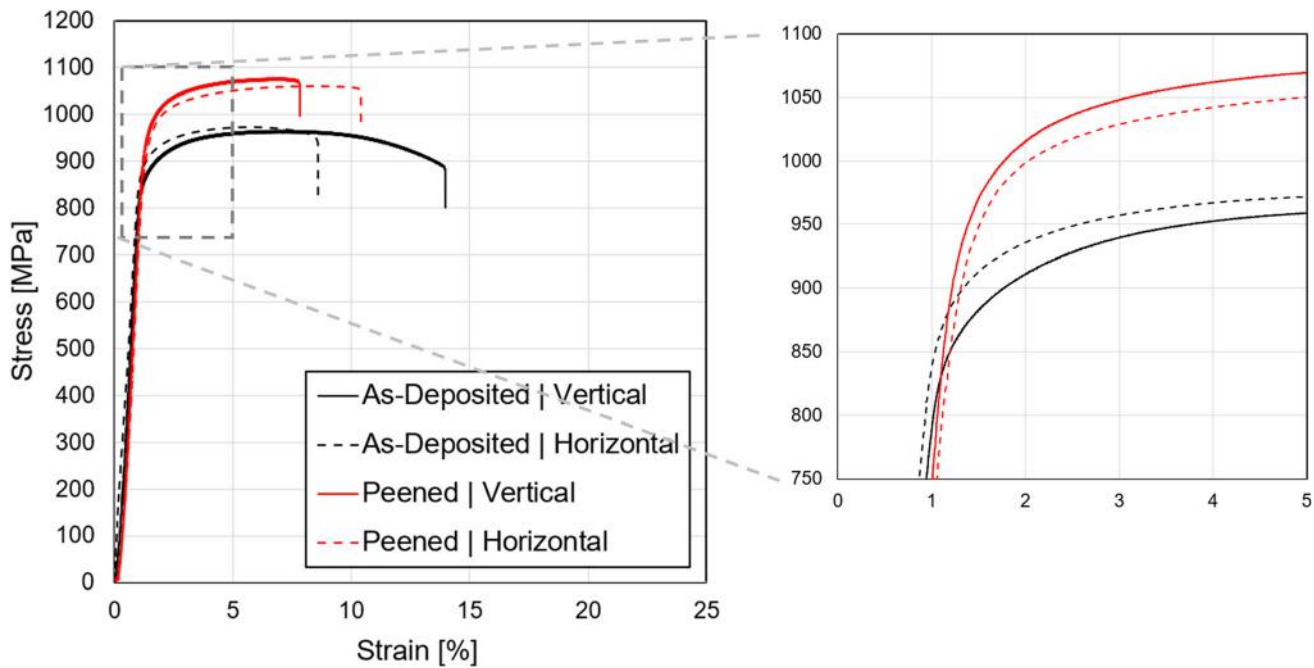


Fig. 10—Comparison of tensile engineering stress-strain curves for the Ti6242 WAAM samples tested in horizontal and vertical directions (parallel to WD and ND) for as-deposited columnar and peened equiaxed grained samples.

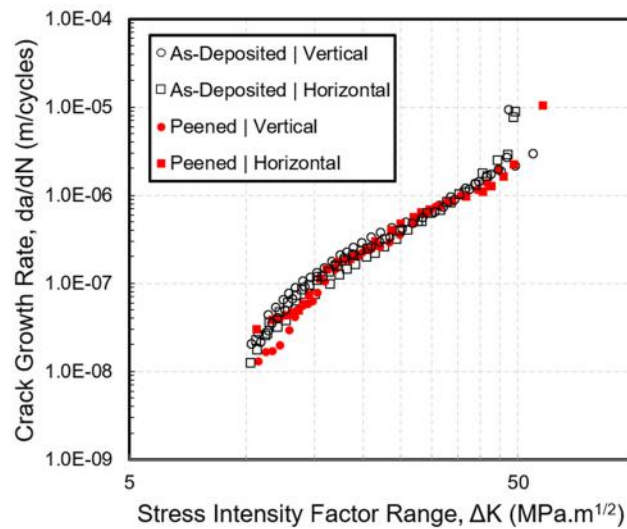
being maintained with each parent β grain, there is an abrupt change in the microtexture of the tri-variant colony orientation sets between neighbouring β grains. In addition, in ND, HAZ bands are apparent where the transformation microstructure has been influenced by repeated passes of the heat source during layer deposition. This generates rapid heating cycles with peak temperatures in the range of $\sim 850^\circ\text{C}$ to below the β transus ($\sim 1000^\circ\text{C}$ ^[18]), causing α -lath coarsening through the partial dissolution and regrowth of α . However, very close to the β transus, the small amount of residual α that remains stimulates the formation of a thin band of larger single variant α colonies on cooling, due to autocatalytic nucleation that is biased by the last remaining α variant in a given region.^[18,40,50] The peak temperature gradient thus causes HAZ bands with a cyclic, 'saw tooth'-like variance in the inter-lamellar spacing in the build-height direction, combined with a strong microtexture band at its upper limit, formed by single variant colonies (previously discussed in depth in References 14, 17, 18). Examples of these systematically spaced HAZ bands have been highlighted in the α -phase EBSD map in Figure 3(c) (and also in Figure 12).

The last large-scale heterogeneity in the transformed $\alpha + \beta$ microstructure is caused by GB α allotriomorphs with attached single-variant colonies that develop on some, but not all, of the columnar β GBs as long bands. Along specific β GBs a continuous dual α layer with a single orientation is formed, with neighbouring aligned single-variant-orientation laths growing out into the parent β grain. These laths have a diffuse interface with the multivariant colony regions within the parent β -grain interiors due to the interpenetration with laths

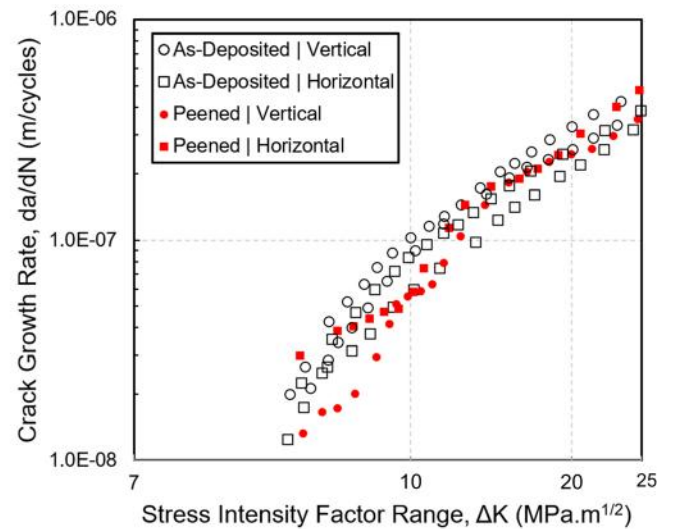
of other orientations nucleated within the β grain, or growing inwards from other β GBs. The term 'GB α ' will be used henceforth to collectively describe this single α orientation dual layer.^[40,51]

Examples of GB α layers in a columnar β -grain sample can be seen in the example α -phase EBSD maps in Figure 3(c) (and also in Figure 12) covering large lengths of the β GBs in the Ti64 and Ti6242. These GB α bands generally only form at higher angle columnar GBs, where the GB α nucleates with an orientation relationship with one of the parent grains and they develop first at low undercooling when the transformation structure starts to form during cooling from above the β transus. Comparative BSE micrographs and EBSD maps of an example GB α layer in a columnar prior- β Ti64 grain structure are shown in Figure 5. They consist of parallel $\alpha + \beta$ lamellae with similar crystallographic orientations (~ 5 deg misorientation) growing into each grain from the GB with a different lath growth direction either side of the prior- β GB with a 95° between them. However, their appearance and apparent width is strongly influenced by the metallographic sectioning plane. Due to the high cooling rate in AM, each of these single variant colonies has only been able to grow to $\sim 100\ \mu\text{m}$ in width before impinging with the multivariant colonies forming within the grain. Since the GB α crystallographic orientations are dictated by the BOR there is only a small orientation difference between the colonies either side of the GB, as shown in the pole figures in Figure 5(d).^[15,40] The laths of the GB α can be seen to interweave with the surrounding multivariant microstructure.

Ti64

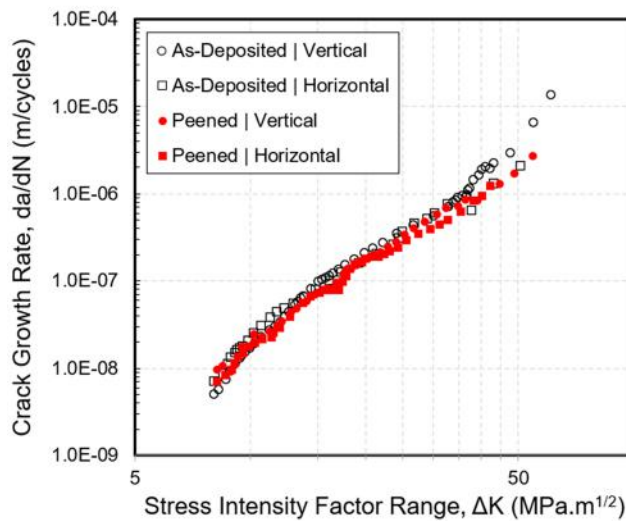


(a)

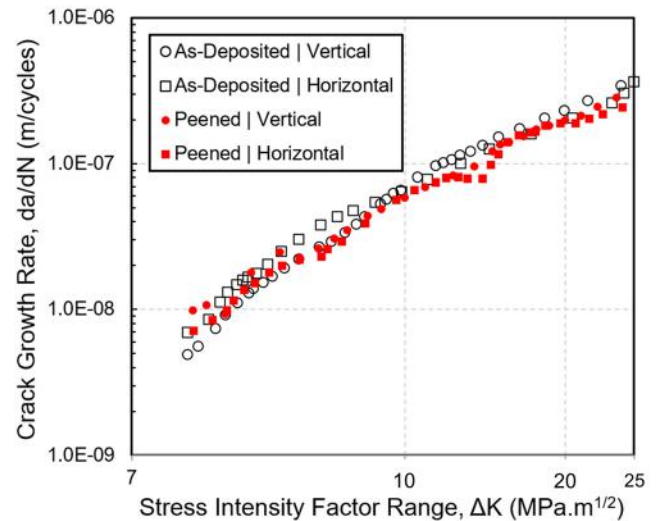


(b)

Ti6242



(c)



(d)

Fig. 11—Crack growth rate plotted against stress intensity factor range, for as-deposited (columnar grains) and peened (equiaxed grains) samples, for (a, b) Ti64 and (c, d) Ti6242. (b, d) show the $< 25 \text{ MPa m}^{1/2}$ ΔK region magnified to clarify the extent of growth rate anisotropy and data scatter in the crack regime most affected by the sample microstructures (please note the different y-axis scales).

The α laths within the interior of the WAAM parent β grains have a finer lamellar spacing and colony size than in wrought products due to the large β -grain size and the much higher cooling rate experienced during WAAM deposition ($\sim 30 \text{ }^\circ\text{C/s}$ ^[18]). The α laths in the as-deposited Ti64 and Ti6242 samples were measured to have an α inter-lamellar spacing of ~ 1.0 and $\sim 0.7 \text{ }\mu\text{m}$, respectively^[21] (measured between HAZ bands) as shown in Figure 6(a) and (e); *i.e.* the Ti6242 transformation microstructure was finer than for Ti64, which is expected for the difference in alloy composition, where molybdenum in Ti6242 retards the α growth rate.^[21]

2. Equiaxed β -grain WAAM structures

For comparative purposes, inter-pass peening has been employed to build Ti64 and Ti6242 WAAM samples with refined β -grain structures, which are shown in the optical macrograph and reconstructed- β EBSD maps in Figure 7. These samples exhibited equiaxed β grains homogeneously throughout the regions used for mechanical testing and, although the processing conditions were designed to produce as similar grain structures as possible, they had slightly different average grain diameters of 277 ± 6 and $266 \pm 5 \text{ }\mu\text{m}$, respectively. The textures of the grain-refined samples are shown in the pole figures in Figures 4(e) and (f) and

exhibit significant β -phase texture weakening when compared to the columnar grain samples; *i.e.* for Ti64, the columnar grain sample texture strength was reduced from 23.6 to 1.8 MRD by inter-pass peening (though it should be noted that the columnar grain texture is likely exacerbated somewhat by the limited number of sampled grains). This much weaker texture is subsequently passed onto the α transformation microstructure, also producing very low intensities of ~ 2 MRD in the Ti64 and Ti6242, which is weaker than exhibited by conventionally produced wrought products [52–54].

In the conventional coarse and columnar grain material, GB α single variant colony layers appear in 2D sample cross sections as long bands decorating the prior- β GBs aligned approximately parallel to the build-height direction (*e.g.* Figure 5). In contrast, in the peened material, as the columnar grain structure was replaced with near-equiaxed grains with no preferential alignment and generally higher grain-to-grain misorientations, a much less directional network of GB α is created that reflects the more isotropic GB topography. Examples of which can be seen in the correlative EBSD and BSE images in Figure 8. It is also now more obvious, due to the larger number of GBs sampled, that the apparent width of the GB α layers vary considerably due to the sectioning angle in a 2D cross section and that, due to the high cooling rate, the GB α layers are only of the order of 15–35 μm thick.

Within the β grains in the refined peened samples, the transformation microstructure exhibited a similar basketweave tri-variant α colony microstructure of interwoven $\alpha + \beta$ lamellae [Figures 6(c), (d), (f)] compared to in the conventional builds. For a given $\alpha + \beta$ titanium alloy, the transformation microstructure inter-lamellar spacing is controlled by the cooling rate during the final thermal cycle above the β transus during deposition—where it first nucleates—and subsequent high temperature reheating cycles below the β transus,

where coarsening occurs within HAZ bands. Therefore, β -grain refinement did not affect the α lath thickness in these samples, as the thermal conditions during WAAM processing were not changed significantly. The scale of the transformation microstructures in the columnar parent β and refined parent β samples for both alloys are thus comparable and have inter-lamellar spacings of ~ 1.0 and $\sim 0.7 \mu\text{m}$ for Ti64 and Ti6242, respectively. However, it should be noted that if the thermal conditions are not carefully controlled this need not be the case. For example, faster deposition with shorter inter-pass times can result in heat build-up in the deposit and slower cooling rates, coarsening the transformation microstructure (*e.g.* [18] compared to [21]).

B. Mechanical Properties

1. Static testing

Sets of example tensile stress-strain curves for Ti64 columnar and equiaxed β -grain samples, tested in orthogonal ND (vertical) and WD (horizontal) directions, are compared in Figure 9(a). Stress-strain curves for the equivalent Ti6242 samples are shown in Figure 10. The mechanical property results are also summarised in Table IV. Despite having very strong textures, the Ti64 columnar grain samples exhibited an average yield stress (0.2 pct proof stress) of 851 and 802 MPa in the WD and ND directions, respectively, giving a small 90 deg yield-stress anisotropy (vertical/horizontal) of 0.94, which is comparatively better than the data in the literature presented in Figure 1(a) and Table I. This yield-stress anisotropy was entirely eliminated (1.0) in Ti64 by peening the samples during deposition to produce an equiaxed β -grain structure [Figure 7], which also increased the yield stress by ~ 80 MPa. A similar trend is seen for the Ti6242 samples (Figure 10) but the columnar grain samples had very little 90 deg yield-stress anisotropy to begin with (0.97).

Table III. Elasticity and Plasticity Input Parameters for the Crystal Plasticity Finite-Element Simulations

Material	Elastic Moduli [GPa]				
Ti64	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
	160	90	66	182	47
	Basal Slip				
	n_{slip}	a	ξ_0 [MPa]	ξ_∞ [MPa]	h_0 [MPa]
	3	8	310	450	200
	Prismatic Slip				
	3	8	340	450	200
Buffer	Pyramidal Slip				
	12	8	580	850	200
	Elastic Moduli [GPa]				
	C_{11}	C_{12}			
	-0.1	0.001			
	Isotropic Dilatational				
	n_{slip}	a	ξ_0 [MPa]	ξ_∞ [MPa]	h_0 [MPa]
	-	5	0.6	0.3	1

n_{slip} number of slip systems, a stress exponent, ξ_0 initial slip resistance, ξ_∞ saturation slip resistance, and h_0 hardening rate (for interpretation of these values see [47])

More pronounced tensile yield-stress anisotropy (vertical/horizontal) is exhibited in the elongation to failure data of 1.6 and 1.5 for Ti64 and Ti6242 columnar β -grain samples, respectively. The lower elongation to failure exhibited in WD in these samples (and in the literature, Table 1) is a known effect influenced by strain concentrating within the transformation microstructure of particular columnar parent β grains, and for samples with prior- β GBs inclined at high angles to the tensile loading axis (*i.e.* $> \sim 15^\circ$), intense shear localisation can occur in the GB α layers on the columnar β GBs.^[14] Again, peening drastically reduced the elongation anisotropy of the Ti64 and Ti6242 samples to 1.065 and 0.915, respectively, achieving close to isotropy. However, peening also increased the yield stress significantly, which reduced the extent of strain hardening and overall stable elongation and ductility. However, this was only slightly lower than for the worst test orientation of the columnar grain samples.

Finally, an additional Ti64 WAAM experiment was conducted to compare the tensile properties of a sample loaded at 45 deg to the build-height direction [Figure 9(b)]. This 45 deg orientation test exhibited a yield stress ~ 20 pct *higher* than either the horizontal WD or build-height direction, revealing a far worse yield anisotropy of 0.823. This was accompanied by a reduction in elongation to failure to 9 pct resulting in an elongation anisotropy of 0.474. Overall, this dataset has thus revealed the true mechanical anisotropy of columnar grain DED-AM Ti64 WAAM samples that has historically been missed due to the lack of testing at 45 deg to the build-height direction (Figure 10).

2. Fatigue crack growth rates

Fatigue crack growth rate of Ti64 columnar sample data was sourced from Reference 5 for comparison in this work. This dataset included 14 tests on notched samples with cracks propagating in horizontal (WD) and vertical (ND) orientations, extracted from Ti64 WAAM walls deposited with single bead, and parallel and oscillation pass multi-bead deposition techniques, to study the effect of macro/microstructure variability introduced by the AM process on crack growth rates. (Note: these test walls were built continuously; *i.e.* with no controlled inter-pass layer temperature). The results will not be reproduced here in full for brevity. In brief, the fatigue crack growth rate anisotropy was shown to be more pronounced when the stress intensity factor range (ΔK) was $< 20 \text{ MPa m}^{1/2}$, where the growth rates are much more sensitive to the microstructure, with vertically orientated (ND) crack growth rates often between ~ 2 times to an order of magnitude lower when the crack growth rate is $< 5 \times 10^{-7} \text{ m/cycle}$ than when the crack propagates in the horizontal orientation. This was proposed to be an influence of the coarsened α lamellae in the HAZ bands. Notably, the growth anisotropy was much lower for the single-bead WAAM samples in this growth rate regime. However, for both multi-bead depositions studied in Reference 5, 2 out of 8 of the vertical-orientated crack samples exhibited much faster growth rates that were similar to those in the

horizontal orientation. Although the number of tests for this study (and indeed for other similar studies) is too low to ascertain reliable statistics for the growth rate variance, the presence of such high variability, independent of its accurately known probability, is still problematic for safety-critical aerospace applications.

To investigate the impact of refining the parent β -grain structure on crack growth anisotropy and data scatter, further fatigue crack growth data for Ti64 single-bead test walls was generated using samples extracted from the WAAM test walls used for static tensile testing above [Figure 9(a)], built with a controlled inter-pass temperature, with and without machine hammer peening. The full dataset will not be interrogated here (as it will be the focus of a focused future publication), but example data is shown in Figures 11(a) and (b). In the as-deposited condition with columnar parent β grains, for $\Delta K < 25 \text{ MPa m}^{1/2}$ the horizontal crack growth rates were similar to that in Reference 5. However, in the vertical orientation, the growth rates were similar to that in the horizontal orientation in Reference 5 instead of lower, further demonstrating the unpredictable nature of the growth rates in this direction.

The peened samples with equiaxed β -grain structures exhibited high crack growth rate anisotropy between horizontal and vertical orientations in the $\Delta K < 15 \text{ MPa m}^{1/2}$ range. However, the equiaxed β -grain material also demonstrated limited data scatter, with all horizontal and vertical samples (only 1/3 of each shown here) showing little deviation from the average trend (shown in Figures 11(a) and (b)); *i.e.* refining the β grains resulted in *predictable* crack growth rates, although the mechanical anisotropy persisted. As the HAZ banding remains in the peened test samples (shown in the optical macrograph in Figure 7(b)), it may contribute to the crack growth rate anisotropy, where the coarsened α laths in these regions enable higher ductility and could reduce the crack growth rate locally, though this would need to be evidenced (*e.g.* using SEM digital image correlation). Therefore, vertically orientated cracks would encounter many such regions, crossing them perpendicularly, whereas horizontal cracks travel parallel to HAZ bands and can entirely escape their influence. There is also a potential influence of dissimilar residual stress development in as-deposited and peened Ti64 WAAM samples,^[55] thus the complicated nature of fatigue crack growth rate anisotropy requires dedicated future independent study of the contributing factors.

To investigate potential microstructure heterogeneity contributions to the aforementioned crack growth rate data scatter in vertical-orientated columnar grain Ti64 samples, interrupted fatigue tests were conducted, where the tests were halted before complete fracture. EBSD maps from the 3 interrupted test samples in Figure 12 demonstrate the impact of the coarse and columnar grain structure, GB α , and HAZ bands on crack tortuosity. In Figure 12(a), the starter notch was machined near an aligned columnar β GB with a clear GB α layer. Although the crack can be seen to nucleate near the GB ($\sim 40 \mu\text{m}$ away), it then rapidly deflects as it propagates through the single variant GB α colony parallel to the

major axes of the larger laths, which extend out from the GB at an angle of ~ 60 deg, into the surrounding basketweave microstructure [Figure 12(a)i]. The crack then continues to move away from the prior β GB exhibiting the highest deflection of the sample set and tries to bend around to propagate on the plane perpendicular to the loading direction, which results in the greatest crack tip mechanical driving force. It does this with an irregular path as it encounters different multivariant α colony regions. In particular, crack deflection, bifurcation, and high local tortuosity can be seen at some HAZ bands [e.g. Figure 12(a)ii] and certain hard multivariant colonies that are encountered en route [e.g. Figure 12(a)iii].

In contrast, the second crack in Figure 12(b) nucleates within the basketweave matrix right beside a GB α layer on a prior columnar β GB [Figure 12(b)i]. It then propagates parallel to the β GB, along the interface between the GB α and the basketweave matrix, with minimal overall deflection. What tortuosity is present arises again at HAZ bands [Figure 12(b)ii] and hard α colonies [Figure 12(b)iii]. In the third sample [Figure 12(c)], the notch was located in the centre of a columnar β grain and, in this cross section, is not near any prior β GBs with a GB α layer. The crack propagates at a vector angled ~ 30 deg away from the build-height direction and minor tortuosity is seen again at some HAZ bands and multivariant α colonies [Figure 12(c)ii]. Although these examples are for 2D cross sections and it is not known what is occurring below the surface, it is still clear that the high length scale heterogeneous distribution of the GB α single variant bands along the prior columnar β GBs and the microtexture variation within grains can have a dramatic effect on the crack-path deflection and the fracture-surface topography. This creates great variability in the local mechanical driving force as well as affecting closure in longer cracks. All of these effects are known to strongly influence crack growth rates.

For inter-pass peened Ti64 WAAM depositions with equiaxed β grains, the heterogeneous GB α that forms on the columnar vertical β GBs often spanning the full

build height is eliminated (e.g. Figure 8), and with it any potential contributions to growth rate data scatter. However, since each deposited layer experiences cyclical heating close to the β -transus temperature, horizontal HAZ bands remain throughout the microstructure (e.g. [20,21]) producing local heterogeneities that have been shown to influence fatigue crack growth. In addition, heterogeneous residual stresses remain in machine-hammer peened WAAM samples.^[55] Therefore, for fatigue crack growth rate tests on Ti64 peened WAAM samples with equiaxed β -grain structures, anisotropy would not be expected to be completely erased. Data for such tests is displayed in Figures 11(a) and (b) and shows the horizontal crack growth rates are initially much faster than that in the vertical orientation—following the trend in the columnar β -grain samples—but after the stress intensity factor range increases past $\sim 13 \text{ MPa m}^{1/2}$, there is a significant improvement in the growth rate isotropy, possibly due to the diminishing effect of local microstructure on the crack propagation with increasing ΔK .

Ti6242 fatigue crack growth rate data is displayed in Figures 11(c) and (d) and shows that the growth rate anisotropy is improved overall when compared to Ti64 [Figures 11(a) and (b)], especially when compared to the data in Reference 5. In the columnar grain samples, initially there is again faster crack growth rates in the horizontally orientated samples compared to those in the vertical orientation, but this is dramatically reduced reaching near-isotropic growth rates after $\sim 13 \text{ MPa m}^{1/2}$, similar to the Ti64 peened samples. The peened equiaxed grain Ti6242 samples exhibit almost no crack growth rate anisotropy at all. The overall reduced crack growth rate anisotropy in the Ti6242 samples may be due to reduced influence of HAZ bands in vertically propagating cracks, since the cyclic ND variance of α inter-lamellar spacing is less prominent in Ti6242 than in Ti64 due to the slower diffusing molybdenum solute restricting grain growth during reheating close to the β transus, which has been demonstrated previously in Reference 21. Unfortunately, due to the complex deformation mechanics that arise from the interaction of

Table IV. Tensile Static Mechanical Properties of the Ti64 and Ti6242 WAAM Samples in the As-Deposited Condition (Exhibiting a Columnar β -Grain Structure) and in the Inter-Pass Peened State (with Equiaxed β -Grain Structures), Where σ_{YS} = Yield Stress (0.2 Pct Proof Stress), σ_{UTS} = Ultimate Tensile Stress, ϵ = Elongation to Failure, WD = Heat Source Travel (Welding) Direction, TD = Transverse Direction, and ND = Build-Height ‘Normal’ Direction

Material	Test Direction	σ_{YS} [MPa]	Max. σ_{YS} Anisotropy	σ_{UTS} [MPa]	ϵ [Pct]	Max. ϵ Anisotropy
Ti64 columnar* [Fig. 9(a)]	horizontal (WD)	851 ± 15	0.943 ± 0.02	922 ± 12	12.1 ± 0.4	0.611 ± 0.170
	vertical (ND)	802 ± 8		887 ± 4	19.8 ± 1.9	
Ti64 equiaxed [Fig. 9(a)]	horizontal	932 ± 15	1.000 ± 0.023	1014 ± 5	10.4 ± 2.5	0.945 ± 0.264
	vertical	931 ± 17		1019 ± 6	11.0 ± 0.8	
Ti64 columnar [Fig. 9(b)]	horizontal	764 ± 29	0.823 ± 0.02	889 ± 11	12 ± 4	0.474 ± 0.269
	vertical	751 ± 4		830 ± 11	19 ± 3	
	45 deg (to ND)	912 ± 10		987 ± 11	9 ± 1	
Ti6242 columnar [Fig. 10]	horizontal	880	0.972	979	8.2	0.656
	vertical	885		952	12.5	
Ti6242 equiaxed [Fig. 10]	horizontal	942	0.998	1056	8.2	0.915
	vertical	944			7.5	

Directional anisotropies were calculated using min/max recorded σ_{YS} or ϵ ratios.*Used for visco-plastic self-consistent simulation CRSS calibration.

microstructure and crack propagation in $\alpha + \beta$ titanium alloys, the mechanisms controlling fatigue crack growth rate anisotropy cannot be investigated more thoroughly with the results presented here. Time-resolved techniques that can probe the slip-system behaviour during cyclical loading, like high-resolution digital image correlation, would be required instead, and will be utilised in the near future.

C. Higher Fidelity Analysis of $\alpha + \beta$ Transformation Microstructure Heterogeneity

Mechanical anisotropy and inconsistent failure behaviour has been linked to the coarse and columnar β -grain structure and related microtexture heterogeneities, such as the HAZ bands and the GB α layers, present in typical DED-AM parts produced in titanium alloys like Ti64, in both the above examples and widely in the literature. The formation of HAZ bands has been studied previously by the current authors and others,^[17,18] but the important GB α layer seen in columnar DED-AM β -grain structures has not been explored in as much depth. To gain insight into the true 3D nature of GB α , its formation, and how it influences mechanical properties as demonstrated above, it is necessary to characterise these complex microstructure regions and the transition to the basketweave microstructure in parent β -grain interiors. In this work, the formation of the Ti64 GB α was observed in-situ in the SEM using a heating stage, to witness its nucleation and growth during cooling from above the β transus ($\sim 980^\circ\text{C}$ ^[18,56]), and its 3D form was studied using plasma focused ion beam (PFIB) serial sectioning with EBSD to reconstruct the 3D morphology of the α variants formed in the β GB region and its transition into the β -grain interiors.

After heating to 1000°C in Figure 13(a), the microstructure of the Ti64 columnar grain sample shows full transformation to β and the mapped EBSD area can be seen to contain 3 large columnar grains, labelled $\beta 1$, $\beta 2$, and $\beta 3$. There is a high-angle GB between $\beta 1$ and $\beta 2$ (18 deg), and a lower angle GB between $\beta 2$ and $\beta 3$ (14 deg). There is also a low-angle GB (10 deg) on the left side of $\beta 1$ that it shares with another columnar grain largely outside the mapping area. The orientations of the β grains are shown in the pole figures in Figures 14(a) and (c). For $\beta 1$ -2 [Figures 13(a)], most of the angles between the crystal poles are high (> 10 deg), however it can be seen in the $\{011\}_\beta$ pole figure that one set of potential α habit planes from the grains $\beta 1$ and $\beta 2$ are close to coincident with an angle of only 4 deg between them. Between $\beta 2$ -3, the overall grain misorientation is lower than between grains $\beta 1$ -2, and a pair of $\langle 001 \rangle_\beta$ poles are closely aligned (< 3 deg).

After cooling the sample to 900°C (26.6 pct indexed α) at approximately 0.3°C s^{-1} (18 $^\circ\text{C/min}$), the α phase can be seen to nucleate at discrete sites on the β GBs in Figure 13(b). This includes the thin layer of allotriomorph that forms along the β GB and α laths that nucleate at discrete points on the β GB and grow

inwards towards the β -grain centres^[40,51] (collectively termed GB α). At this relatively small undercooling and low cooling rate necessitated by the in-situ experiment, the α laths only nucleate along the β GBs and not (heterogeneously) within the β grains. Multiple laths of the same crystallographic α variant nucleate independently but closely separated on the β GBs, often on both sides of the GB, with the same orientation. These subsequently form the templates for single variant α colonies that develop as the temperature drops, by transforming the retained β within the same α variant within their sphere of influence, by branching, and by autocatalytic variant selection.^[40,50]

After cooling to 750°C the $\beta \rightarrow \alpha$ phase transformation was mostly completed (63.3 pct indexed α) and the colony skeletons can be seen to have 'filled in' in Figure 13(c) until only thin films of β remain in between, producing single-variant colonies of parallel α lamellae consisting of a single variant.^[40] However, the size of the colonies formed at the 2 highlighted β GBs are different. At the $\beta 1$ -2 GB [Figures 13(d) and (e)], single-variant colonies ($\alpha 1$ and $\alpha 2$) form both sides of the β GB and cover nearly all of its length in the mapped area. The laths either side of the β GB in Figure 13(b) grow approximately perpendicular to each other (73 deg angle between them), which is a common trait of this type of colony (*e.g.*^[51]). Both colonies have adopted orientation variants where their $[0001]_\alpha$ poles match the overlapping $\langle 011 \rangle_\beta$ poles of their parent grains $\beta 1$ -2 through the BOR (highlighted in Figures 14(a) and (b)), though their $\langle 11\bar{2}0 \rangle_\alpha$ poles match independent $\langle 111 \rangle_\beta$ directions from each adjoining parent β grain, exhibiting an 8 deg angle between them. Micromechanically, the formation of this type of single variant colony can be approximated as a single α 'grain' that straddles a β GB, is $\sim 380\ \mu\text{m}$ wide, and extends into the columnar grains on both sides. (Note: the GB α in Figure 13 is larger than that in the as-deposited WAAM samples ($< 150\ \mu\text{m}$ wide) due to the much lower undercooling that had to be employed during the in-situ experiment).

In comparison, at the $\beta 2$ -3 GB [Figures 13(b) and (c)] several α colonies form in competition with different orientation variants, covering short sections of the GB length each. In the higher magnification maps in Figures 13(f) and (g), at 900°C it can be seen that different initial α lath variants are nucleating at different points on the same boundary. Similar to colonies $\alpha 1$ -2, $\alpha 3$ -4 adopt a variant matching the orientation of the closest $\{011\}_\beta$ poles of the neighbouring parent grains $\beta 2$ -3, maintaining the BOR, as shown in Figures 14(c) and (d). Conversely, the colonies labelled $\alpha 5$ -6 [Figures 13(f) and (g)] exhibit no shared poles across their neighbouring parent β grains $\beta 2$ -3, and instead maintain the BOR independently in each grain [Figure 13(e)]; but due to the low misorientation of the parent β grains, they still have a reasonably low misorientation of 12 deg between them.

Overall, these results show that GB α single-variant colony formation is heavily influenced by small variations in β grain-to-grain misorientations and the local environment the α laths nucleate in (*e.g.* by autocatalytic

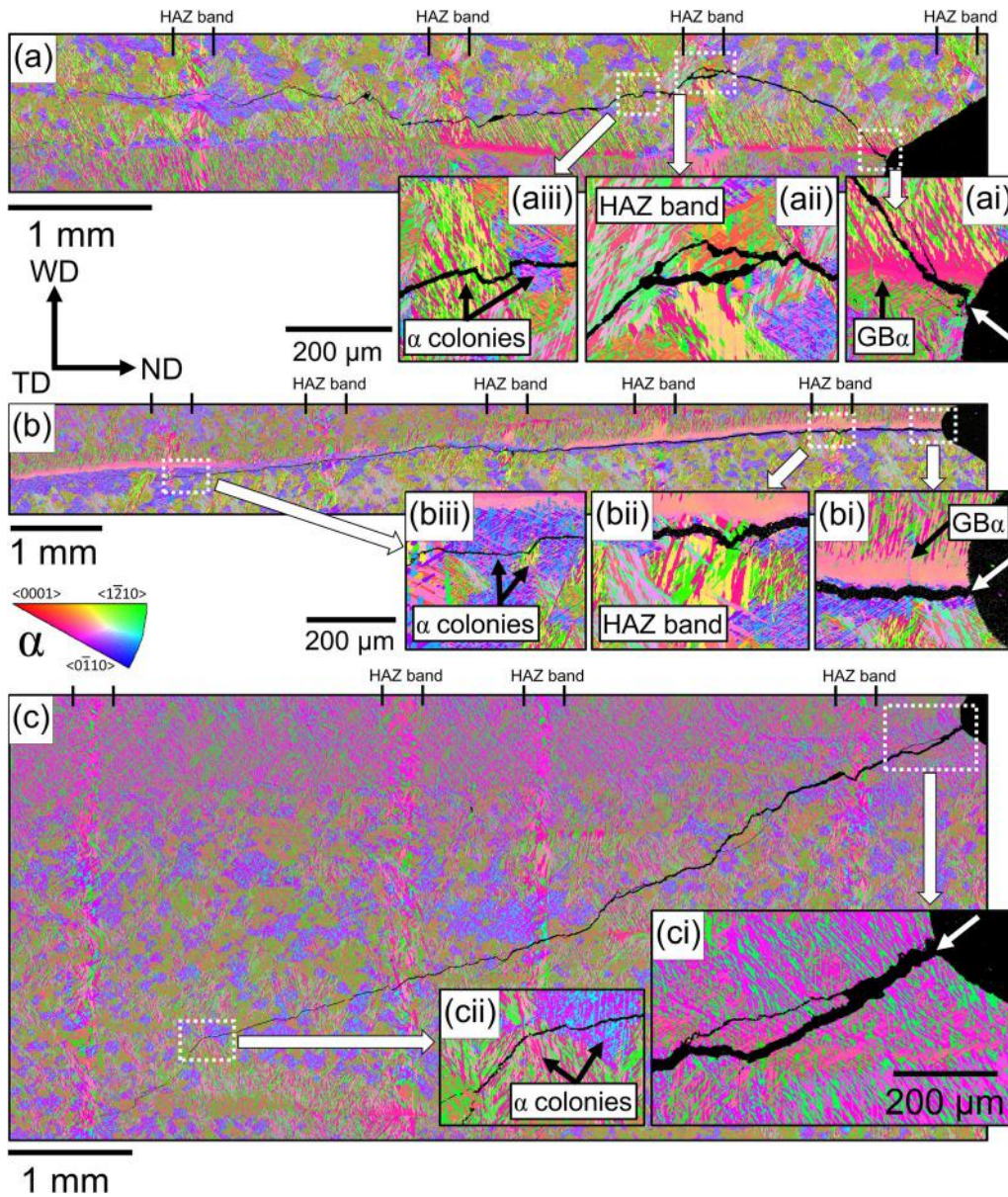


Fig. 12— α -phase EBSD maps of interrupted fatigue crack growth test samples, showing the influence of microstructure heterogeneity on crack growth behaviour.

nucleation), resulting in inconsistent formation of large $GB\alpha$, corroborating with previous studies with different β -phase textures.^[40,51] These results are included here to highlight the seemingly paradoxical unpredictable and persistent nature of large $GB\alpha$ formation— β -grain misorientations are not possible to control during AM-process solidification to any practical degree (and indeed neither can the β GB plane orientations that have also been suggested to be influential^[51,57]), therefore identifying $GB\alpha$ -susceptible β GBs are extremely difficult to predict within $\alpha + \beta$ titanium alloy microstructures. Furthermore, due to the $GB\alpha$ dependency on the parent β -grain structure that cannot be altered without additional thermomechanical processing, post-deposition β -annealing heat treatments are unable to prevent

the large single-variant colonies reforming upon subsequent cooling through the β transus, which has been demonstrated in a previous study.^[40] This persistency results in irremovable large $GB\alpha$ in the microstructure.

To better understand the 3D morphologies of the $GB\alpha$ microstructures, a $\sim 250 \times 200 \times 100 \mu\text{m}$ volume was extracted from the Ti64 WAAM material shown in Figures 3(a) and (c), using a femtosecond laser and PFIB equipped SEM, across a typical prior- β GB and then serially sectioned with each slice scanned by EBSD. The full reconstructed volume is shown in Figure 15(a) where the microstructure is segmented using a > 2 deg boundary misorientation criterium (coloured randomly). A large layer of α with a single variant orientation can be seen to straddle the former β GB in

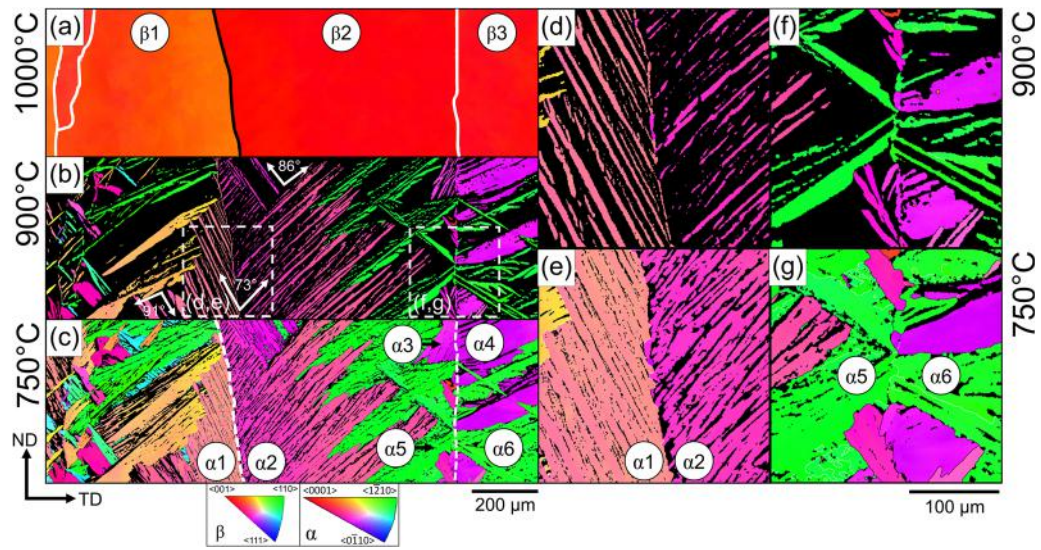


Fig. 13—EBSD results from the in-situ heating SEM experiment carried out to directly observe the formation of GB α microstructures in a WAAM Ti64 sample by cooling from above the β transus temperature: (a) the starting columnar β -grain structure directly indexed at 1000 °C, (b, c) α phase growing from the GB seen at 900 °C (26.6 pct indexed α) and 750 °C (63.3 pct indexed α). Magnified regions of interest are shown at (d, f) 900 °C and (e, g) 750 °C.

the central region of the analysed volume, which fully fills the space and extends further as discrete laths into the β -grain interiors where it interpenetrates with other variant orientations to form a typical multi-variant basketweave microstructure. The segmented single-variant GB α volume has been isolated and shown separately in Figure 15(b) in greyscale band contrast (EBSD pattern quality) to better define the $\alpha + \beta$ lamellae boundaries. This confirms that a central 50 μm -wide (in TD) section consists completely of a single α orientation, with no penetration from other α laths of different orientations. However, either side of this region, laths of the same variant orientation extend outwards on both sides in TD. Although these appear lath-like in 2D metallographic cross sections (*e.g.* Figures 6(a) and (b)), the 3D rendering demonstrates that they are highly irregularly shaped and are better described as having a plate morphology.

Further smaller segmentations in the vertical ND-TD (i–iii) and horizontal WD-TD (iv–vi) planes are shown in Figures 15(c) to better depict the morphology of the GB α . Pseudo-2D cross sections are also provided in Figures 15(d) and (e) to highlight the growth direction of the α laths either side of the prior β GB. Although the prior β GB was slightly curved, it can be seen to be approximately parallel to WD, and the α lath growth directions on the left and right sides are all consistently tilted ~ 75 and 25 deg, respectively, away from WD, and have an angle of ~ 100 deg between them. On the right side of the β GB, the α lath growth direction is orientated ~ 45 deg away from ND and the prior β GB.

In Figure 16, further examples of basketweave α grains have been segmented to show how they interact with the GB α , and how they align morphologically with the WAAM reference directions. Figures 16(a) and (b) show grains either side of the GB α (where (a) is rotated

180 deg around ND with respect to (b)). The individual basketweave grains have been subdivided into large interwoven and irregularly shaped grains (left in Figures 16(c) and (d)) and into smaller grains that exhibit more well-defined shapes (right). All of these latter grains reach the extracted volume edge, so their full size cannot be determined from the current dataset. Nevertheless, they provide valuable insight into the growth directions of the basketweave grains. Like the lamellae extending out from the GB α , the other α variants in the basketweave region have irregular plate-like morphologies tilted at high misorientations to ND, WD, and TD. It is apparent that these complex 3D-morphological trends must be taken into consideration alongside crystallographic orientations when discussing deformation mechanics in DED-AM $\alpha + \beta$ titanium alloys.

Since the 3D volume analysed contained a low number of α grains due to practical limitations, large-area 2D cross sections were analysed instead to investigate morphological global trends in Ti64 WAAM. This was achieved by collecting 10 mm ‘lines’ of BSE images (333 images for each) of the $\alpha + \beta$ lamellar microstructures from the samples shown in Figures 3(a) and (b) and Figure 7(a), for columnar and equiaxed parent β -grain structures respectively, which were then processed using bespoke code to extract the orientations relative to ND of all α ‘lath’ long axes (more details in §2.2). For the columnar sample, where the image line scans spanned multiple parent β grains, the collected data [Figure 17(a)] shows that, overall, the relative frequency of lath long axes peaks at approximately ± 40 deg relative to ND (~ 80 deg between the peaks) and there is local minimum parallel to ND, agreeing closely with results published previously by Liu *et al.*^[58] on electron beam-wire DED-AM Ti64. Given

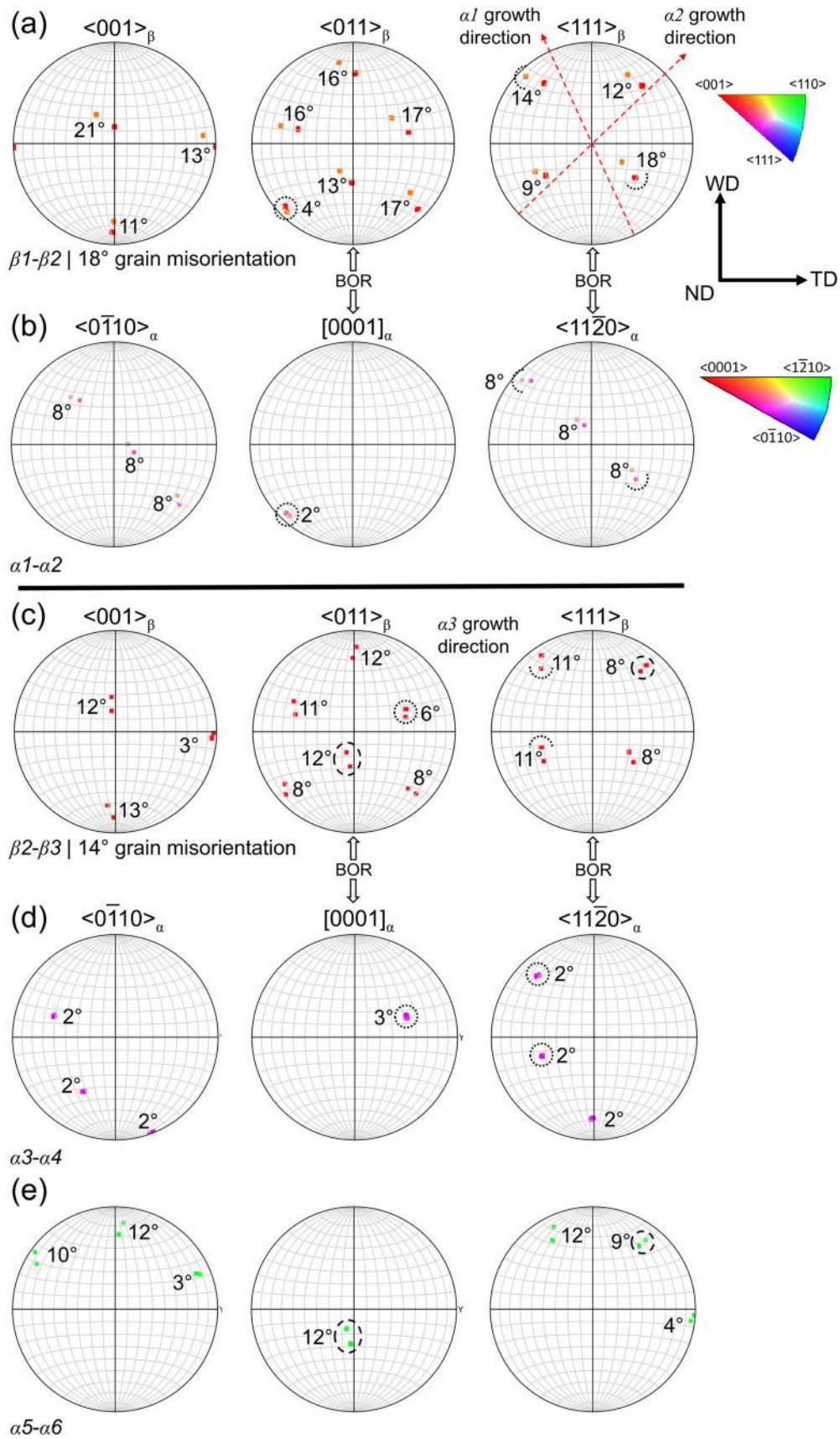


Fig. 14—Pole figures displaying the orientations of β and α grains of interest shown in the in-situ heating SEM experiment in Fig. 13. (Note: pole figure projected plane matches the plane of the EBSD scans).

many parent β grains were sampled for our analysis, it is strong evidence for a global trend of the microstructure.

For the equiaxed grain sample, data from 3 parent β grains of interest have been segmented and collected in Figure 17(b) for clarity. *Parent grains 1* and 2 show similar dual peaks in their angular distribution to the columnar grain sample, which are also near orthogonal, but at different grain rotations relative to ND—*Parent Grain 1* has peaks at -65 and 21 deg, parent grain 2 has peaks at -55 and 45 deg. *Parent Grain 3*, interestingly, exhibited only 1 peak at -15 deg, which is perhaps due to the cross sectioning. Nevertheless, it would appear that the equiaxed microstructure produces similar intra-grain orientations of α laths when viewed in 2D, but these bear no relation to the WAAM build direction, which is a proposed influence of the very weak β texture [Figure 4(e)].

D. Crystal Plasticity Simulations

To aid investigation of the microstructure and texture influences on mechanical properties, full-field crystal plasticity (CP) modelling was employed. Several uniaxial tensile test simulations were conducted using the DAMASK^[47] and MatFlow^[49] packages, in ND, TD, and 45 deg to ND test orientations, using idealised synthetic grain structures to represent different combinations of α grain morphology and texture strength. These also included representing the material conditions analysed above by importing EBSD data into the simulations for:

- (i) A ‘worst case scenario’ of a transformation α microstructure and *strong* texture extracted from an α Ti64 EBSD map dataset for a columnar parent β -grain [e.g. Figure 3(a)], segmented from a *single* transformed parent β grain containing numerous α laths of sufficient resolution for accurate deformation simulation (EBSD step size of $0.25\ \mu\text{m}$, Figures 18(b) and (g)).
- (ii) A Ti64 transformation α microstructure with *weak* texture from a refined equiaxed parent β -grain microstructure (grain diameter $\sim 50\ \mu\text{m}$) from WAAM samples produced with inter-pass deformation simulation^[34] [Figures 18(d) and (i)].

The simulated stress-strain curves for the idealised grain structures and texture cases are shown in Figure 19 and the predicted yield-stresses are summarised in Table V. Importantly, it can be noted that when using a synthetic simple equiaxed grain α microstructure [Figure 18(a)] with the transformed α texture taken from the single parent β -grain [Figure 18(g)], which had an α strength of 32 MRD, little yield-stress anisotropy was observed between ND and TD orientations, which is perhaps surprising. This weak yield asymmetry is a result of the cubic symmetry of the BCC β phase and the strong $\langle 001 \rangle_\beta \parallel$ ND texture that is inherited by the α transformation microstructure through the BOR, which leads to

similar crystallographic alignment of the α orientation variants with respect to the orthogonal WAAM reference directions in ND and TD when there is no significant variant selection.^[60]

Overall, the CP simulations with equiaxed α grains and strong texture could not replicate the larger asymmetry seen in the Ti64 WAAM experimental results in Figure 9, predicting only a small increase in yield stress for the 45 deg loading orientation, resulting in a yield-stress spread across all loading directions of only 35 MPa. Further simulations were therefore performed where the equiaxed α grains were replaced with the lamellar α microstructure imported from EBSD map data obtained from the columnar Ti64 samples. The results of these simulations are shown in Figure 19(b), where it can be noted that, with a lamellar WAAM α microstructure, the 45 deg loading orientation case has now led to a larger difference relative to ND and TD of 65 MPa. These predictions, which now include the lamellar microstructure, are much closer to that seen in the experimental results for Ti64 in Figure 9(b). This therefore suggests that the microstructure morphology plays an important role in producing the experimentally measured yield-stress anisotropy, even though the local constitutive model in the CP simulations does not capture the physics of scale, so grain-size dependent strengthening mechanisms are not replicated in these simulations.

When using an equiaxed parent β -grain microstructure with weakened texture as a simulation input [Figures 18(d), (e), (h), (i)], the tensile loading produced little yield stress anisotropy, with a difference of only 15 MPa in all loading orientations. The stress-strain curves for this simulation are shown in Figure 19(c). The simulation also captured the yield-stress increase seen in the experimental data of tested samples with these microstructures (e.g. Figures 9a and 10); i.e. if compared to the simulation in Figure 19(b), there is a ~ 60 MPa increase for TD and ND loading orientations. However, interestingly, the 45 deg to ND yield-stress simulation for the columnar parent grain simulation input is much closer to that of the equiaxed parent grain microstructure. The implications of these CP simulation results will be discussed below.

IV. DISCUSSION

A. Impact of β -Grain Structures on Yield-Stress Anisotropy

Published data (Figure 1, Table I) consistently shows a trend of yield-stress anisotropy in DED-AM Ti64 tensile test samples with coarse and columnar prior β -grain structures, where the horizontal (WD/TD) yield stresses are higher than the vertical test orientation (ND). For example, the stress-strain curves of the Ti64 samples tested in this work (Figure 9) showed slight yield-stress anisotropy between ND (build-height direction) and WD (welding/heat source travel direction), where the WD yield stress was 49 MPa higher. However, the additional Ti64 test set [Figure 9(b)] at 45 deg

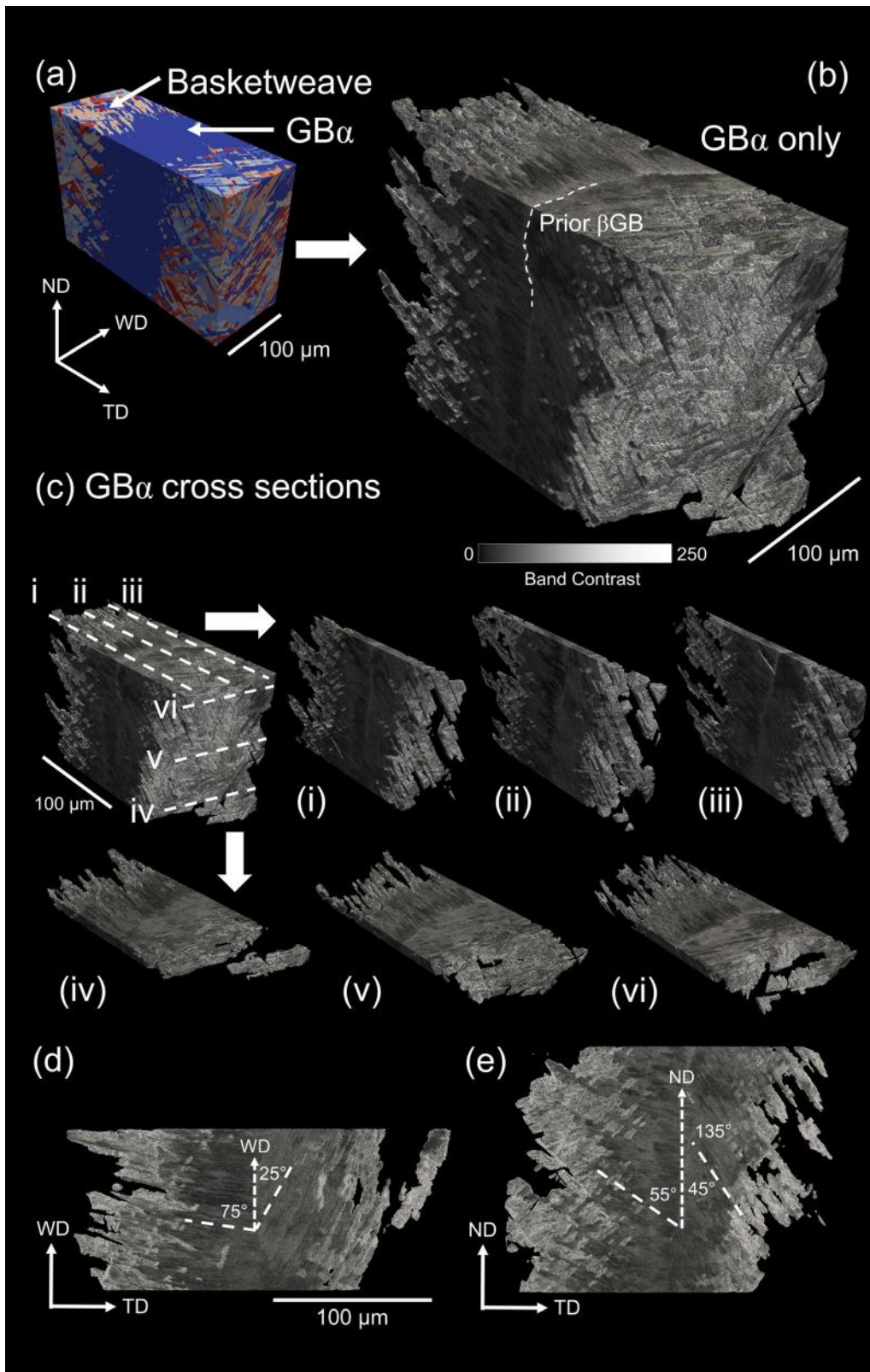


Fig. 15—3D images of a typical grain boundary α (GB α) region formed across a β GB in a Ti64 WAAM sample reconstructed by EBSD: (a) the whole segmented block consisting of the GB α and 'matrix' basketweave α laths (colours assigned randomly to each grain), (b) the segmented GB α single variant colony displayed with EBSD band contrast, (c) cross sections of (b) in orthogonal planes, (d, e) analysis of α lath growth directions in orthogonal planes.

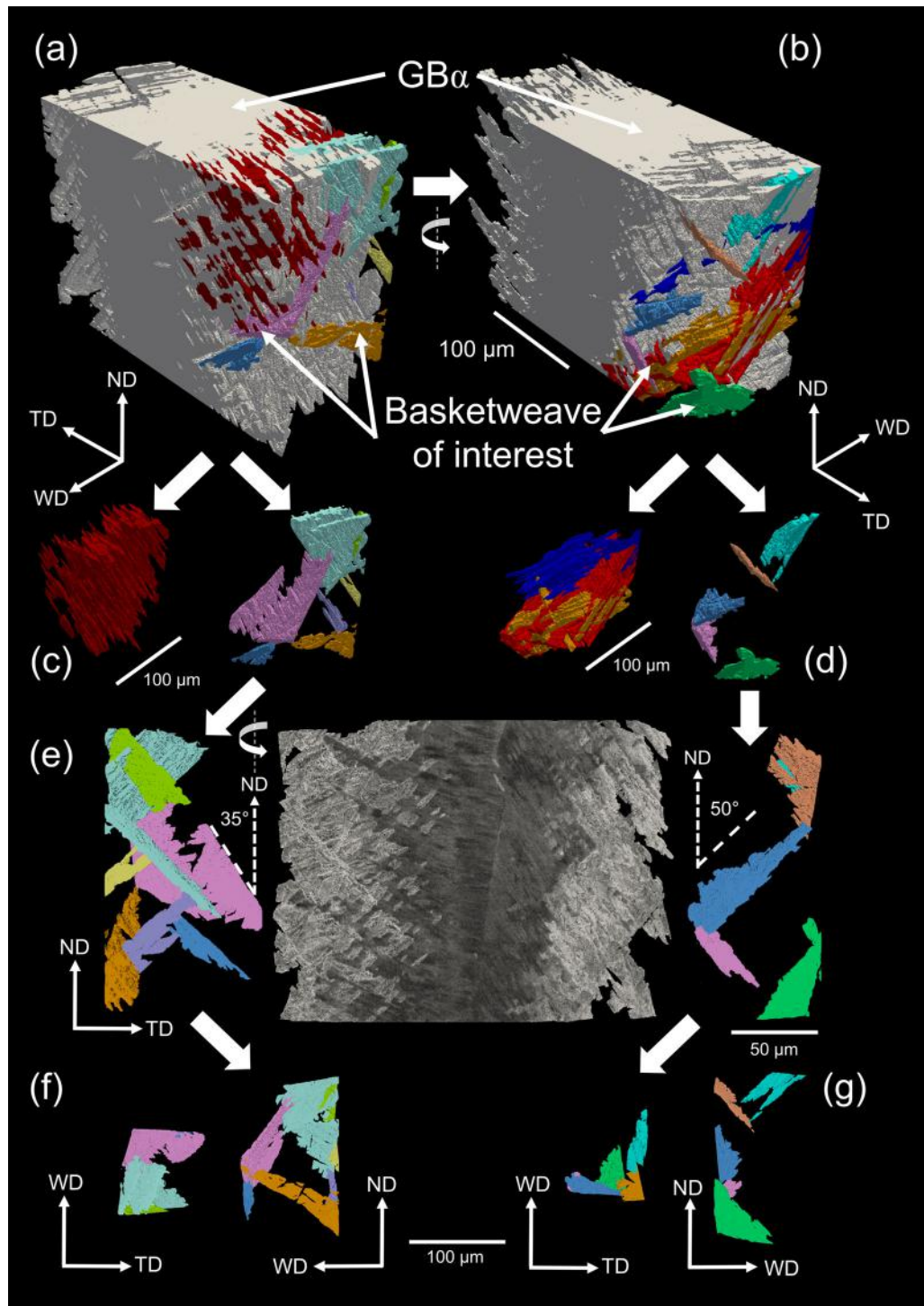


Fig. 16—3D EBSD images showing (a, b) the interaction of the grain boundary α with the surrounding basketweave microstructure, and (c, g) the morphological alignment of the basketweave laths with the WAAM reference frame.

from ND (around TD) exhibited a much more significant yield-stress anisotropy with a 160 MPa increase in yield stress compared to ND. Strong textures are known to promote yield-stress anisotropy, particularly in HCP metals, *e.g.* strong $[0001]_z \parallel$ TD textures seen in wrought Ti64 products.^[15,59] However, the effective slip line

length (the distance dislocations travel before arresting) is also a known factor to influence the yield stress.^[15] The spatial alignment of the transformation microstructures [Figures 15, 16, 17] in $\alpha + \beta$ titanium alloys formed from coarse and strongly textured columnar parent β -grain structures must therefore also be taken

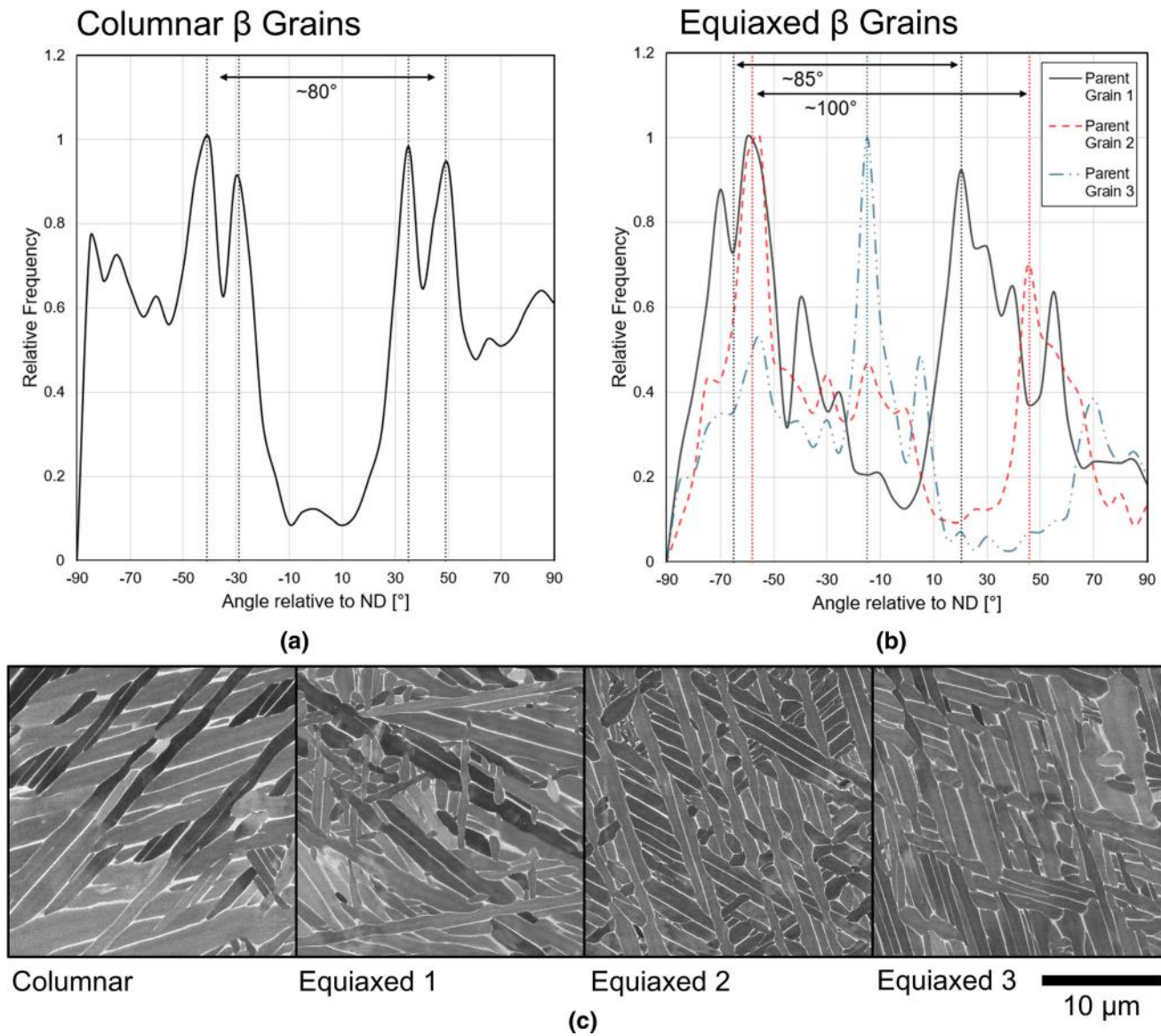


Fig. 17—Relative frequency plots of orientations of α lath long axes relative to the build direction (ND) extracted from SEM backscatter electron images of 2D cross sections taken from (a) columnar and (b) equiaxed parent β grain samples. (c) Example images from each dataset shown in (a) and (b).

into consideration when determining sources of yield-stress anisotropy.

1. Columnar β -grain structures

CP simulations were used to investigate the effect of both microstructure and texture on yield-stress anisotropy in Ti64 WAAM samples. In the columnar parent β grain samples, there are symmetric angular distributions in the α pole figures [Figure 18(g)] that are produced by the BOR from the cube orientated parent β -grain texture, which represent many orientations with high Schmid factors that can accommodate basal and

prismatic slip in the α transformation microstructure. This is demonstrated in the combined basal and prismatic Schmid factor maps in Figures 20(b) and (d) used for CP simulation input, where the high Schmid factor values are shown to be distributed homogeneously throughout the microstructure for both ND and TD loading directions. This leads to relatively homogeneous simulated strain distributions [e.g. Figure 20(c)] that lead to lower symmetric yield stresses for orthogonal ND and TD load cases when the $\langle 001 \rangle_{\beta}$ crystal poles are closely aligned with these directions. Additionally, the highest strain concentrations are seen in

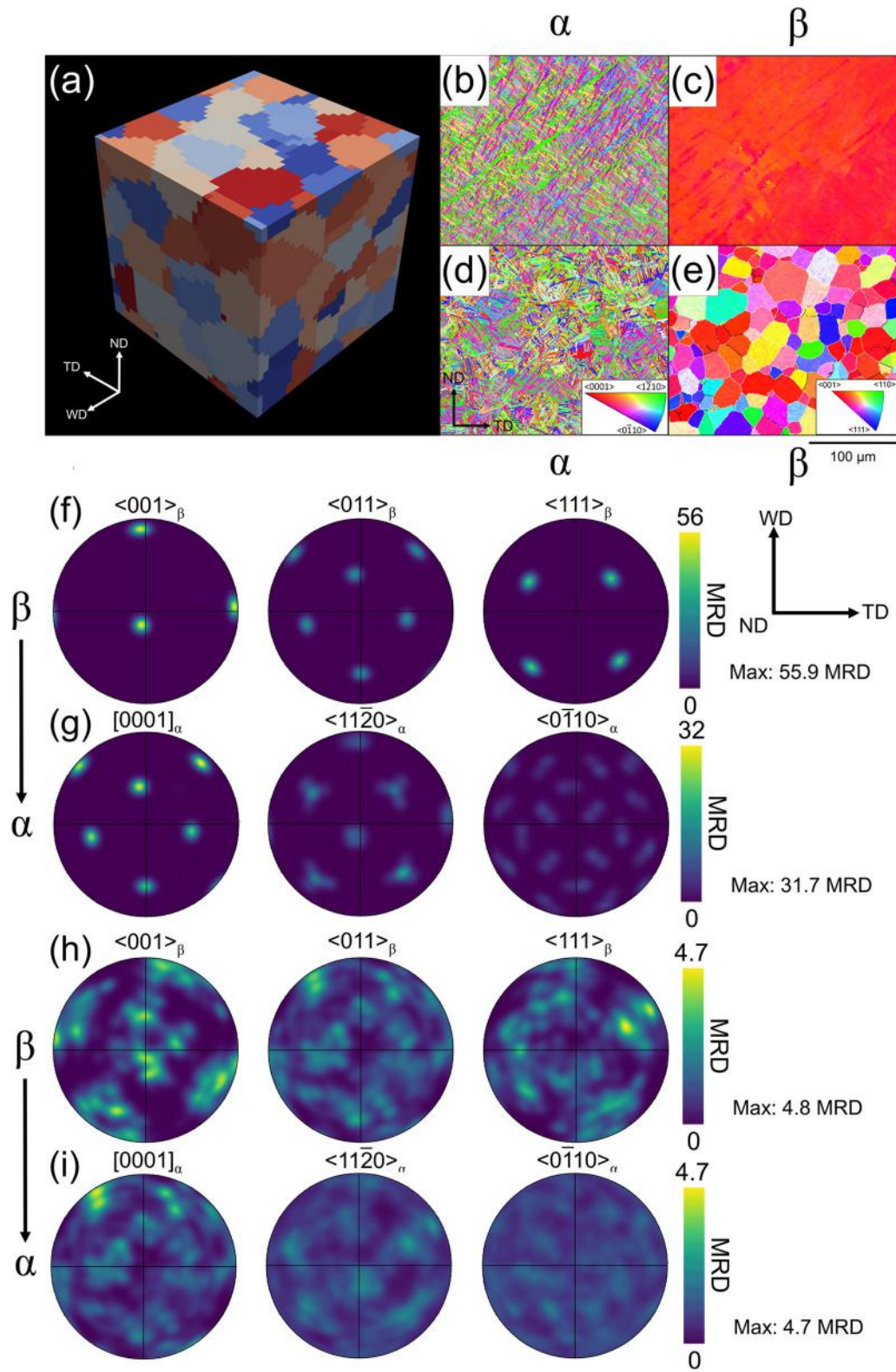


Fig. 18—Ti64 microstructures and textures used in crystal plasticity simulations: (a) synthetic equiaxed grain microstructure, (b) α -phase EBSD transformed from the single β grain shown in the reconstructed- β EBSD in (c), (d) α -phase EBSD transformed from the polycrystalline parent β WAAM microstructure shown in the reconstructed- β EBSD in (e); (f) texture for the single β grain, (g) α texture produced upon transformation from the β -phase texture in (f), (h) texture for the polycrystalline β WAAM microstructure, (i) α texture produced upon transformation from the β -phase texture in (h).

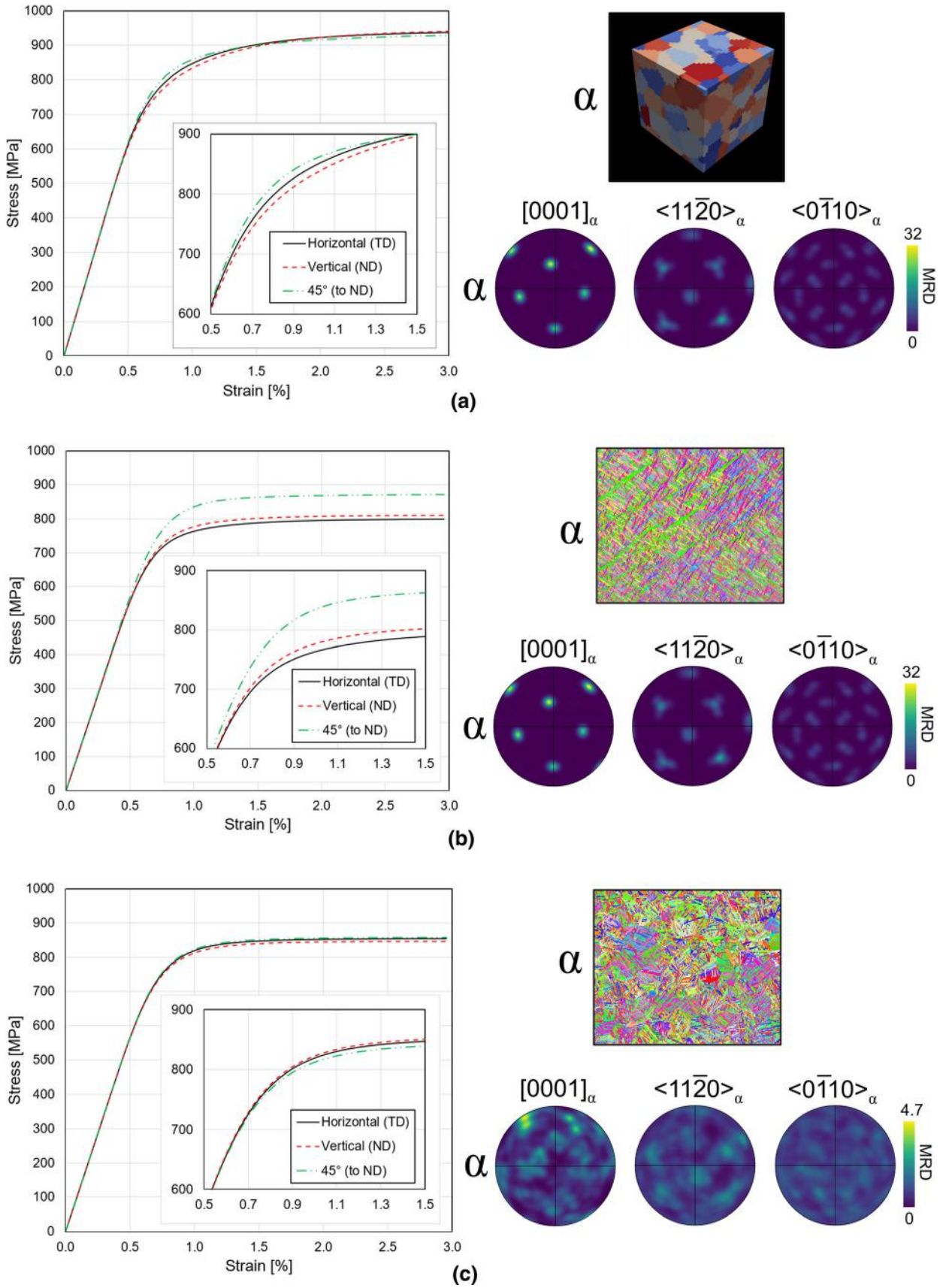


Fig. 19—(Left) Simulated stress-strain plots of Ti64 WAAM tensile tests using full-field crystal plasticity modelling with (right) the various inputs from Fig. 18: (a) using Figs. 18(a) and (g), (b) using Figs. 18(b) and (g), (c) Figs. 18(d) and (i).

high-Schmid-factor laths with their long axes aligned ~ 45 deg to ND and TD; *i.e.* those aligned closely with the maximum resolved shear-stress orientation.

However, in the 45 deg loading orientation [Figures 20(e) and (f)], there are fewer high-Schmid-factor laths for basal and prismatic slip, which show some correlation to tri-variant colony distribution as seen in the IPF map in Figure 20(a), resulting in more heterogeneous strain distribution. This is particularly noticeable in the higher magnification insets that show that the longer laths orientated at 45 deg to ND/TD accommodate little strain, and strain instead concentrates discontinuously largely in the very soft variant laths that are often surrounded by unstrained harder variants.

In the α microstructure used for the columnar parent β -grain loading simulation [Figure 18(b)], it can be seen that there is a tendency for the 2D cross-sectioned α laths to be elongated ~ 45 deg to ND/TD. A similar analysis was conducted here on BSE images in the ND-WD plane [Figure 17], which shows the frequency of cross-sectioned α lath major-axis orientation with respect to ND has a clear maximum at $\sim \pm 40$ deg. When tensile loading these α microstructures in ND or TD/WD orientations, the highest resolved shear stress will thus be aligned near-parallel to the majority α lath long-axis orientation at 45 deg to ND, resulting in a maximised slip line length without the need for slip transfer across lamellar plate boundaries, which is approximated in the CP simulations with continuum-based stress equilibrium throughout the volume element.

Conversely, when loading at 45 deg to ND or TD, the slip line length is parallel to ND/TD/WD, which is more closely aligned to the majority α lath *minor* axis and so is minimised, restricting dislocation movement and accelerating grain hardening and stress transfer. Because of the aligned slip systems within single variant colonies, slip transfer is known to be relatively easy in lamellar titanium microstructures.^[61] However, this will be more difficult in multi-variant basketweave microstructures where different orientation variants will reduce the slip line length in a given volume, which will increase the strength of this effect relative to that seen in single α variant colony microstructures found in fully lamellar β -annealed wrought components. This is, of course, an oversimplification of plasticity behaviour in Ti64 basketweave microstructures, but, overall, the biasing of the microstructure morphology with a high frequency of lath alignment with the shear plane would be expected to impede dislocation movement less and result in a lower yield stress.

The CP simulations of the lamellar basketweave microstructures when loading parallel to ND and TD also demonstrate that strain tends to concentrate in the high-Schmid-factor soft laths with the longest major axis orientation at 45 deg to ND [Figures 20(b) and (c)]. With minimised obstructions to shear presented by different lath variants along the maximum resolved shear stress orientation in the microstructure, ND and TD loading simulations present with relatively low yield stresses when compared to the same simulations run with the equiaxed (synthetic) grain structure (Table V).

For the 45 deg loading simulation, the maximum resolved shear stress orientation is parallel to ND and TD, and so simulated shear is often obstructed by harder lath variants, which produces the discontinuous strain concentrations in the strain map in Figure 20(f). When this effect is combined with the reduced number of soft laths for simulated basal and prismatic plane shear, the simulated yield stress is increased.

Therefore, it can be concluded that the ‘morphologically biased’ α microstructure contributes strongly to the yield-stress anisotropy on top of that resulting from the strong transformation α texture. Furthermore, the very large tensile yield-stress anisotropy for DED-AM Ti64 (or similar $\alpha + \beta$ titanium alloys) with coarse and columnar parent β -grain structures is not revealed without testing loading directions orientated 45 deg to the orthogonal AM reference directions, and this is a direct result of the strong $\langle 001 \rangle_\beta \parallel$ ND solidification texture.

2. Equiaxed β -grain structures

Refining the columnar β -grain structures in DED-AM $\alpha + \beta$ titanium alloys was shown above to completely remove both yield-stress and elongation anisotropy (in orthogonal ND and WD/TD orientations) but also lead to a higher yield stress (Figure 9). β -grain refinement radically weakened the β texture and resulted in a near-texture-free α transformation microstructure (*i.e.* the α texture in the Ti64 WAAM samples reduced from 13.3 to 2.4 MRD), and randomisation of the parent β texture would appear to produce no preferential physical alignment of the α plates in the transformation microstructure when averaged over multiple grains [Figure 17(b)]. There is thus no contribution from geometrical alignment of the lamellar microstructure or α texture on yield asymmetry in the peened samples with equiaxed parent β -grain structures. Even though the bulk mechanical properties of the peened samples are now isotropic, it still does not lead to homogeneous grain-scale plasticity. Each β grain can only produce a set of 12 (maximum) α crystal orientations through the BOR during cooling below the β transus^[15,60] and the grain size in refined DED-AM $\alpha + \beta$ titanium builds is still typically hundreds of microns in diameter. Therefore, each individual parent β grain will still contain its own α microtexture an order of magnitude larger than the microplasticity activity (*i.e.* each lath-to-lath slip interaction) and GB α layers are still present on the GBs. However, with an equiaxed prior- β microstructure, microtextured α grains will be much more isotropically dispersed throughout the macro/microstructure leading to less slip concentration at prior β GBs.

For studies using alloy modification to refine the β -grain structure, the yield stress increase can be often partially attributed to solid solution strengthening or other changes to the microstructure, such as the scale of the α , related to the specific alloy elements used. For grain refinement methods not using alloy modification (*e.g.* inter-pass deformation), overall, yield-stress increases of up to 150 MPa have been reported that can only be attributed to the change in β -grain structure

Table V. 0.2 Pct Yield-Stress and Anisotropy Data Summary for the Crystal Plasticity Simulations

α Microstructure	α Texture Type and Strength	Max. σ_{YS} Anisotropy	σ_{YS} [MPa]			
			TD	ND	45 deg to ND	ND
Equiaxed (3D, Fig. 18(a))	single parent β grain, α strength = 31.7 MRD [Fig. 18(g)]	0.958	815	795		830
Single parent β grain, lamellar α (Pseudo 3D, Fig. 18(b))	single parent β grain, α strength = 31.7 MRD [Fig. 18(g)]	0.921	755	755		820
Polycrystalline parent β , lamellar α (Pseudo 3D, Fig. 18(d))	polycrystalline parent β , α strength = 4.7 MRD [Fig. 18(i)]	0.981	805	810		795

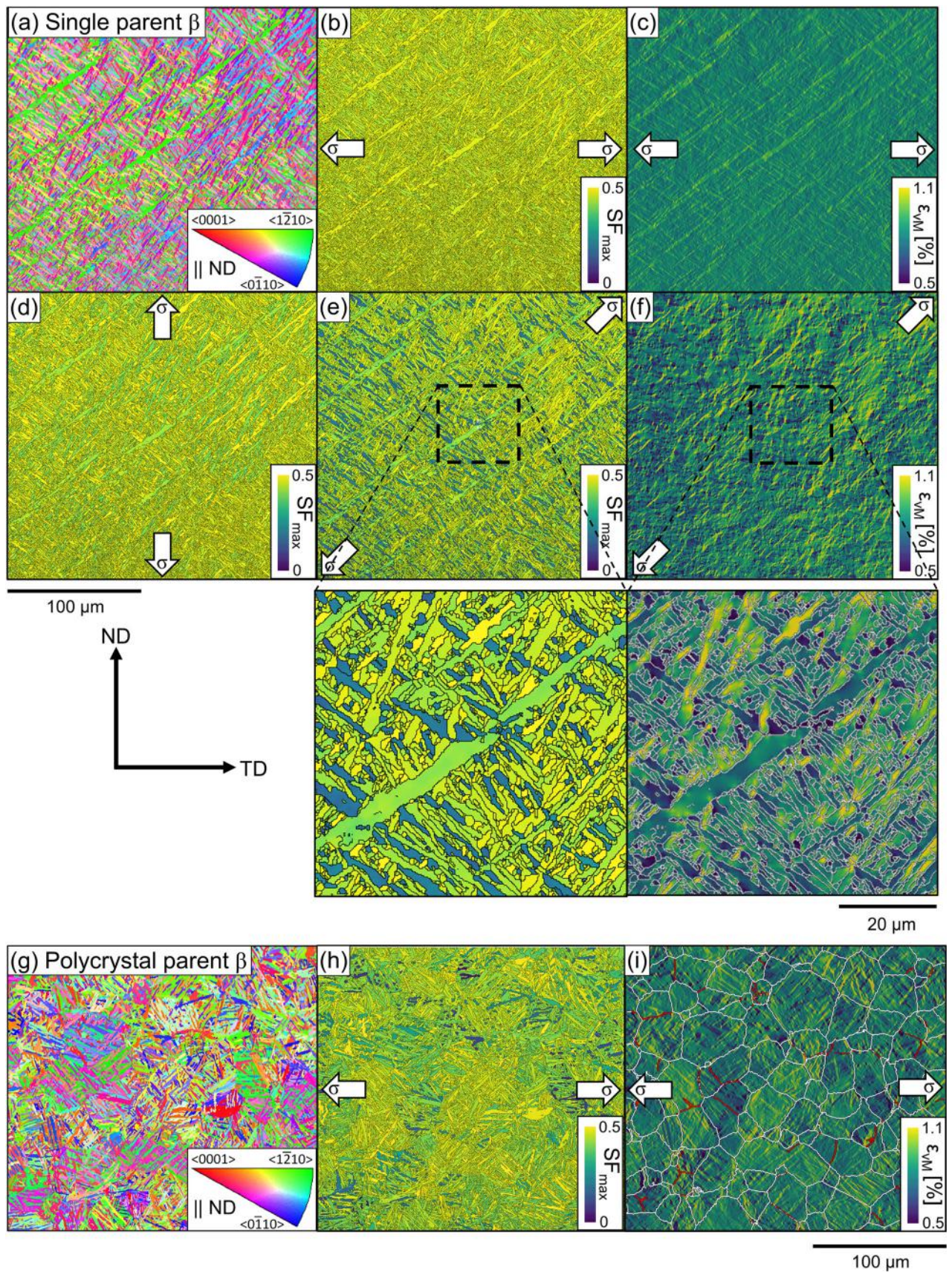
Maximum yield-stress anisotropy was calculated using the ratio of lowest-to-highest values for the loading directions tested

Fig. 20—Comparison of simulated strain in α microstructures inherited from single β grain and polycrystalline parent β structures, at a bulk strain of 0.9 pct: (a–f) single parent β grain, (g–i) polycrystalline parent β structure; (a, g) α -phase EBSD maps, (b, d, e, h) max Schmid factor value maps, relating to the indicated loading direction, for both basal and prismatic slip, (c, f, i) simulated strain maps. High and low-angle grain boundaries are highlighted in white and red, respectively, in (i).

and/or the transformation microstructure.^[16,20] However, the greater yield stress cannot be attributed directly to a reduction in β -grain size as the β grains are far larger than the slip line length in the transformed α ^[14,62]—which is related to the lamellar colony size—and is ill-defined in a multivariant lamellar microstructure, but largely independent of the β -grain size being mainly controlled by the cooling rate.

For inter-pass deformation processes, the extra time taken to peen or roll a deposited layer can allow the substrate of previously deposited material to reach a low enough temperature to increase cooling rates during deposition throughout the build, refining the transformation microstructure inter-lamellar spacing when compared to a part built more quickly without inter-pass deformation, leading to an increase in yield stress. However, the Ti64 tensile tests reported in this study (Figure 9) were made with samples machined from WAAM material produced with carefully controlled substrate temperatures to produce consistent inter-lamellar spacings with and without peening,^[20,21] and still show a yield stress increase within the same margin reported in the literature. Therefore, the greater yield stress increase is a real effect that must be related to another direct consequence of refining the β -grain structure.

The strong $\langle 001 \rangle_{\beta} \parallel \text{ND}$ β texture with 45 deg aligned α laths in columnar Ti64 samples actually gives the lowest yield stress for orthogonal vertical/horizontal loading, as it has more soft-orientation variants than from a random distribution and also provides easier slip paths at the orientation of highest resolved shear stress. Therefore, the equiaxed β -grain structure that has weak texture and averaged α plate alignment would naturally provide a higher and more isotropic yield stress linked only to the β -grain refinement. The CP simulation results concur with this assessment [Figures 20(g) and (i)], showing significant heterogeneous strain concentration correlated approximately to regions with higher combined basal and prismatic slip Schmid factors, and/or within laths that have their major axis orientations near to 45 deg relative to the loading direction. The stress-strain curves for simulated loading of this microstructure show isotropic yield stresses across ND, TD, and at 45 deg to ND, which all also exhibit a yield stress increase of ~ 50 MPa when compared to ND/TD loading of the columnar parent β -grain microstructure facsimile, correctly replicating the experimental data behaviour [Figures 9 and 10] and the literature.^[16,20] However, a higher fidelity microplasticity study of refined DED-AM $\alpha + \beta$ titanium alloys is required to fully understand the hardening mechanisms involved.



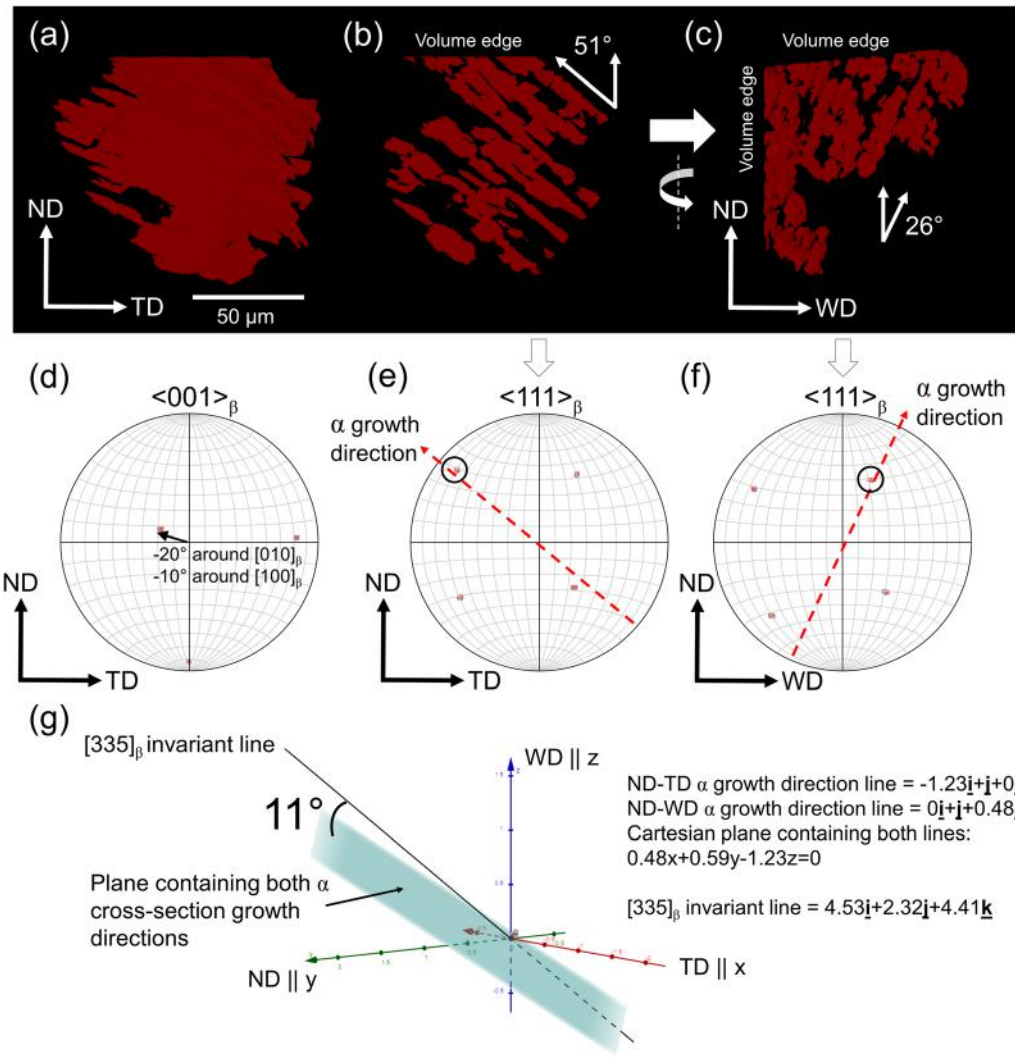


Fig. 21—(a) 3D reconstruction and (b, c) thin 2D cross sections of the large α grain shown in Fig. 16(c); (d–f) pole figures of interest showing the reconstructed parent β -grain orientations related to the α major growth directions shown in (b, c); and (g) showing the orientation of a plane calculated to contain the α growth direction lines and its orientation relative to the closest invariant line of the parent β grain.

3. Formation of GB α and morphologically aligned transformation microstructures

β phase related morphological alignment of the α transformation microstructure has been shown to be important in determining the yield stress and yield asymmetry in lamellar titanium AM materials. However, the thin GB α single variant lamellar colonies seen in AM microstructures that ‘straddle’ the prior- β GBs, while being too small in volume fraction to have a great effect on the yield stress, are also of great interest because they are known to strongly influence slip localisation and failure process (e.g. Figure 12).

The in-situ SEM heating experiment in Figure 13 revealed that single variant GB α colonies are formed progressively when cooling below the β transus by individual, separated, α laths nucleating first along both sides of the β GBs. Once these first laths form, they grow out into the grains either side of the β GB and more nucleation occurs at less viable sites as the undercooling

increases. It has been proposed that neighbouring α variants with the same orientation nucleate autocatalytically on a particular side of the β GB as the elastic strain field exerted on the surrounded β at a GB can be relaxed by nucleation of the same α variant.^[40,50] This results in the residual β being progressively filled in by more α laths as the temperature drops until a continuous layer is developed along the GB surface. However, because they develop in a falling temperature condition and nucleate at different undercoolings, they are able to grow different distances into the grain before impingement. Early laths that nucleate on other grain faces will thus be able to deeply penetrate into partly transformed skeletal colonies, and other α variants that nucleate later within the grains as the undercooling increases will penetrate less far. This creates a diffuse interwoven interface with the basketweave microstructure seen in the grain centres. It may also be possible that tri-variant colonies can nucleate autocatalytically from subsets of

the 12 variants possible by the BOR from dislocations within the grains. 3D sectioning here has now shown that the transformed α is far more interconnected than previously realised, and the lamellae conventionally seen in 2D sections are actually formed by larger, complex, branched single α plates in 3D.

In the WAAM material with columnar grain structures, the same single variant orientation is more frequently adopted straddling the β GBs than in a randomly textured isotropic grain structure. It has been proposed that colonies seen in wrought grain structures occur because it is energetical favourable for α laths to nucleate from the same point on either side of the β GB if they share a common habit plane in both parent grains.^[50,51] In a columnar WAAM grain structure composed of neighbouring coarse and columnar β grains within the $\langle 001 \rangle_\beta \parallel$ ND β fibre texture, there is a high probability of $\langle 001 \rangle_\beta$ alignment such that it is possible for the same α variants with a $[0001]_\alpha \parallel \langle 110 \rangle_\beta$ OR to nucleate more commonly on both sides of a β GB. Unless there is a marginal benefit for nucleation between two variants, a single variant will thus frequently nucleate either side of a columnar GB along a considerable length, as there is little change in the characteristics of a GB plane between two columnar grains over large distances. These GB α colony layers can therefore be uniquely observed over linear distances that span centimetres throughout the material, following the columnar β GBs in ND (e.g. in Figures 3(b) and 12(b)). As seen in Figure 12(b), if located at a crack initiation site with favourable loading conditions, this large length-scale linear heterogeneity can lead to the development of very straight and more-rapidly growing fatigue cracks. By refining the parent β -grain structures, the β GBs are shorter in length and orientated randomly (as shown in Figure 8), leading to shorter lengths of GB α forming at a variety of angles relative to the preferred crack-path vector, which would, overall, produce more predictable crack propagation behaviour.

Another key aspect of WAAM transformation microstructures, which affects their yield asymmetry, is the propensity for the α laths to growth at angles near to 45 deg to the β texture fibre axis, both when nucleating at GBs and within the grain interiors. This phenomenon has also been observed previously^[40,51,63] and is caused by the lath growth directions preferentially aligning with the invariant line formed between the α and β phases, which is orientated 14.4 deg from the $\langle 111 \rangle_\beta / \langle 11\bar{2}0 \rangle_\alpha$ crystal directions ($\langle 3\bar{3}5 \rangle_\beta$). For example, the pole figures for the β grains $\beta 1$ -2 featured in the in-situ SEM heating experiment [Figure 14(a)] show that the GB α 1 and 2 growth directions marked on the $\langle 111 \rangle_\beta$ pole figure align within ~ 15 deg of the poles; i.e. near-parallel to the α - β invariant lines. It should be noted that the α laths are not needle-shaped when considered in 3D and are more closely approximated as irregularly shaped plates or discs with high aspect ratios, as shown in Figure 15. In 2D they can appear as laths with a variety of angles between them depending on how the feature is cross sectioned.^[51] The interface plane

between α and β is also created by structural ledges with the BOR and $\{0001\}_\alpha \parallel \{110\}_\beta$ habit plane maintained on each step, and it is possible for it to deviate from the invariant line by adjustment of the ledge spacing by some degree.^[63] Nevertheless, as shown in Figures 13, 14, the β texture will still bias the α laths to preferentially form with growth directions at a ~ 45 deg precession to ND in DED-AM $\alpha + \beta$ titanium alloy samples with strong $\langle 001 \rangle_\beta \parallel$ ND fibre textures, as the α - β invariant lines would commonly be orientated close to this angle.

However, the 3D dataset reveals that there is more complexity to the α transformation microstructure than previously acknowledged. To investigate preferred growth directions in 3D for α grains nucleating within parent β grains away from the GBs, the largest continuous single α variant region captured in the 3D-EBSD dataset was analysed [large red grain in Figure 16(c), also shown in Figure 21(a)]. This grain (and indeed others in Figure 16) appears to consist of interconnected thin 'sheets' stacked atop one another. When it is viewed instead as orthogonal thin cross sections [Figures 21(b) and (c)] this sheet-like morphology is clearer and shows there are preferential growth directions in the ND-TD plane orientated ~ 51 deg from ND (around WD), and also in the ND-WD plane orientated 26 deg from ND (around TD). Each sheet 'section' is not discrete and many can be seen to join up through perturbations from the sheet plane. The orientation of the parent β grain (determined from the EBSD dataset) is shown in the pole figures in Figures 21(d) through (f) with these preferred α growth directions projected onto them, showing there is close alignment with the $\langle 111 \rangle_\beta$ poles, which are 14.4 deg from the invariant lines. However, such an analysis is not sufficient when considering the 3-dimensionality of the system. Thus, the cartesian plane of the 2 extracted preferred growth directions was determined (i.e. from the vectors in Figures 21(b) and (c)) and was compared to the closest invariant line of the reconstructed parent β orientation. This analysis shows that the invariant line was orientated ~ 11 deg to the preferred growth plane. Given the error introduced by the experimental method where it is difficult to maintain accurate alignment between the images and crystallographic directions, and other factors such as the influence of phase-transformation-induced strain and competition for space with other α grains (e.g. the GB α) on the most energetically efficient interface plane, this small deviation adds credence to the theory that the α - β invariant lines significantly influence the growing α during the $\beta \rightarrow \alpha$ phase transformation.

Therefore, the strongly textured parent columnar β -grain structures in DED-AM $\alpha + \beta$ titanium alloys would morphologically bias the room-temperature α transformation microstructure enough to introduce the yield-stress anisotropy reported above. Refinement of the parent columnar β structure and heavily reducing the texture strength (e.g. Figure 4) would randomise the invariant line orientations, prevent any α morphological bias globally, and eliminate the yield-stress anisotropy.

V. CONCLUSIONS

Mechanical property anisotropy of directed energy deposition AM $\alpha + \beta$ titanium alloy samples (Ti64 and Ti6242 WAAM) was investigated at length using data available in the literature and from new experiments. Columnar parent β -grain structures and equiaxed grain structures were compared to elucidate the impact of refining the parent grain structures on the mechanical anisotropy. The key conclusions are summarised below.

- Both the literature and current results show that there is a trend of minor yield-stress anisotropy in DED-AM Ti64 samples with columnar parent β -grain structures, which are generally only tested parallel and orthogonal to the AM build direction. It has been revealed that this common testing practice hides the true yield-stress anisotropy, and it was shown that a test orientation rotated 45 deg away from the build direction gave rise to a yield stress ~ 20 pct higher than parallel or orthogonal test orientations.
- The cause of the above yield-stress anisotropy was investigated with crystal plasticity simulations. This suggested that not just the parent β and child α textures were responsible for the anisotropy, but also an α -microstructure lath-orientation biasing, whereby the α -lath long axes were preferentially orientated at a ~ 45 deg rotation away from the AM build direction, influencing the plasticity behaviour and resultant yield stresses. This microstructure morphological biasing was also seen in 3D microstructure datasets.
- Refining the parent β -grain structure heavily reduced the texture and randomised the lath orientations, eliminating the yield-stress anisotropy completely in crystal plasticity simulations. The texture weakening and α lath orientation randomisation also led to an overall increase in yield stress when compared to columnar grain samples.
- The continuous and long grain boundary α colonies that form on columnar β -grain boundaries during the $\beta \rightarrow \alpha$ phase transformation were demonstrated to have a strong impact on fatigue crack growth tortuosity, whereby their influence can cause cracks to travel parallel to the prior β -grain boundaries with little deflection. These cases would therefore have accelerated crack growth, and due to the relatively large spacing of these α colonies in the DED-AM microstructure, would lead to significant crack growth rate data scatter. Importantly, the formation of these detrimental heterogeneous grain boundary α colonies is challenging to predict, and they are persistent; *i.e.* they cannot be removed by post-AM-build heat treatments.
- Since equiaxed β -grain parent structures do not have millimetre-scale near-straight boundaries, the grain boundary α colonies that form are discontinuous and relatively small, and therefore their influence on large-scale fatigue crack growth rates is removed, eliminating the data scatter seen in columnar grain samples, which was confirmed experimentally. However, crack growth rate anisotropy was found to persist when the parent β -grains were refined in Ti64.

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CONFLICT OF INTEREST

On behalf of all the authors, the corresponding author states that there is no conflict of interest.

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The impact of columnar and equiaxed -grain structures on mechanical anisotropy in high-deposition-rate additively manufactured + titanium alloys

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