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Three-dimensional modeling and simulations of single-crystal and bi-crystal titanium for high-strain-rate loading conditions

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Abstract: High purity single crystal titanium (Ti) under shock wave loading is modeled under both one-dimensional and three-dimensional cylindrical conditions. Cylinder sizes of 10 μm and 20 μm radius are both considered in order to assess influence of boundary conditions. A thermodynamically consistent single crystal model for application to shock conditions is presented. The model accounts for the coupled non-linear elastic, dislocation slip, deformation twinning, and structural phase transformation response of the titanium material. Plate impact experiment results using a copper flyer are used to compare against the simulations for crystals oriented in $[0001]$ and $[10\bar{1}1]$ crystallographic directions. The one-dimensional and three-dimensional simulations of the two differently oriented single crystals indicate differences between the one-dimensional and three-dimensional representation, especially for the $[10\bar{1}1]$ oriented single crystal. This orientation breaks the relative orientation symmetry between the crystal and cylinder which otherwise exists for the $[0001]$ oriented single crystal. A significant amount of heterogeneity in the field response of the $[10\bar{1}1]$ oriented simulation was demonstrated due to the highly coupled nature of the deformation. A bi-crystal model composed of both the $[0001]$ and $[10\bar{1}1]$ orientations with the boundary between the two along the axis of the cylinder is also considered for a cylinder model size of 10 μm . The results indicate a strong

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interaction between the two grains that affects the ω phase volume fraction achieved relative to the single crystal calculations.

Keywords: phase transformation, single crystal plasticity, shock loading, twinning

1. Introduction

Because of its high strength-to-weight ratio, titanium has found broad application in structural systems where weight is a strong consideration. These include many structural components in aerospace systems such as critical components in airframes and engines. Its lightweight nature also makes it amenable for armor application (Mouritz, 2012; Bless *et al.*, 1997; Boyer, 1996; Li *et al.*, 2014; Meyer and Kleponis, 2001; Pettersson *et al.*, 2005; Singh *et al.*, 2017; Sukumar *et al.*, 2013; Tersing *et al.*, 2012). Favorable corrosion resistance and biocompatibility also make titanium an attractive material for medical applications (Aghajanian *et al.*, 2019; Fokter *et al.*, 2017; Ghosh *et al.*, 2019; Khoo *et al.*, 2019; Koizumi *et al.*, 2019). These have been enhanced by the recent advances in additive manufacturing and the prominence of titanium for complex component design (Attar *et al.*, 2018, 2019; Bandyopadhyay *et al.*, 2019; Park *et al.*, 2019; Sheydaeian *et al.*, 2017). For all of these applications the broad knowledge of the mechanical response of the manufactured component is critical. In addition, knowledge of the behavior of the material during processing is required to enable one to achieve desired performance characteristics from the manufactured component (Gao *et al.*, 2019; Hao *et al.*, 2019; Ivanov *et al.*, 2019; Karimi *et al.*, 2018; Yoganjaneyulu *et al.*, 2018). For many of these areas of application and processing conditions, understanding and quantifying the complex deformation response of titanium and its alloys under extreme loading conditions is tremendously important.

Under ambient environmental conditions, high-purity α -phase titanium exists as the low symmetry hexagonal close packed (HCP) crystallographic structure with lattice dimensions $a = 2.9503$, $c = 4.6831$ Å (Boyer and Gall, 1985). In general, there are opportunities for the glide of dislocations to take place on up to five crystallographic systems. Three of these systems are of type $\langle a \rangle$ and two of type $\langle c+a \rangle$, namely Prismatic $\langle a \rangle$ - $\{10\bar{1}0\}\langle 11\bar{2}0 \rangle$; Basal $\langle a \rangle$ - $(0001)\langle 11\bar{2}0 \rangle$; Pyramidal $\langle a \rangle$ - $\{10\bar{1}1\}\langle 11\bar{2}0 \rangle$; and two Pyramidal $\langle c+a \rangle$ systems - $\{10\bar{1}1\}\langle 11\bar{2}3 \rangle$; $\{11\bar{2}2\}\langle 11\bar{2}3 \rangle$ (Balasubramanian and Anand, 2002). In general, dislocation slip is limited to the prismatic systems which offer the lowest energy barrier for motion followed by the

Basal and Pyramidal $\langle a \rangle$ systems (Caillard, 2018) although under dynamic loading conditions that typically result in higher stress magnitudes than quasi-static loading, $\langle c+a \rangle$ slip may occur more readily (Morrow *et al.*, 2016). Dislocation slip is less common on the two Pyramidal $\langle c+a \rangle$ systems as the anisotropy in ease of slip amongst the Prismatic and Basal systems favors twinning modes (Balasubramanian and Anand, 2002; Kalidindi, 1998; Livescu *et al.*, 2019; Salem *et al.*, 2003, 2005, 2006; Song and Gray, 1995a, b). Comparison of energy barrier and ideal shear stresses by using first-principles density functional theory suggests that the favorable slip modes between α and ω phases are different (Kumar *et al.*, 2018)), and we may have different active slip systems between them. This study also teaches about the energetically favorable slip systems in poorly understood ω phase. A Visco-Plastic Self Consistent model was used to describe the texture evolution in $[0001]$ and $[10\bar{1}1]$ oriented single crystals loading dynamically in uniaxial compression (Morrow *et al.*, 2016). It was found that simulations represented the heavily twinned material: the $\{10\bar{1}2\}\langle\bar{1}011\rangle$ tensile twin and $\{11\bar{2}2\}\langle11\bar{2}3\rangle$ compressive twin systems. It was also noted that secondary twinning was observed and is necessary to represent the deformation textures in the two single crystals. An experimental study was performed on polycrystalline high-purity titanium to examine the nature of twinning for differing deformation conditions, with a focus on the early stages of nucleation and growth (Livescu *et al.*, 2019). This study found that three types of twins were observed in the EBSD analysis of the deformed samples: $\{1\bar{2}12\}\langle11\bar{2}3\rangle$ compressive twins, and both $\{1\bar{1}02\}\langle\bar{1}011\rangle$ and $\{11\bar{2}1\}\langle\bar{1}1\bar{2}6\rangle$ type tensile twins. This work forms important guidance in suggesting allowable slip and twinning modes for cases of shock loading conditions as the interest of the work here. Although there is recent work representing deformation twins explicitly for single crystal materials (Ardeljan *et al.*, 2015; Cheng and Ghosh, 2015, 2017; Cheng and Shen, 2018; Chester *et al.*, 2016; Ghosh and Cheng, 2018; Jin *et al.*, 2019), we still largely rely upon homogenized pseudo-slip representation of deformation twinning. The approximation of representing twinning as a pseudo-slip process with volume averaging over the different twin variants is still commonly employed (Beyerlein *et al.*, 2010, 2011; Morrow *et al.*, 2016; Wang *et al.*, 2013). Although twinning is still very much an active research area, we will employ the pseudo-slip procedure (Salem *et al.*, 2003, 2005, 2006) to represent twinning in this work.

For reasons of application and also processing, the phase transformation response of titanium and alloys is also of strong interest (Ao *et al.*, 2019; Kumar and Bag, 2019; Li *et al.*, 2017; Wang *et al.*, 2018). The pathway of $\alpha \rightarrow \omega$ phase transformation in Ti or Zr is very sophisticated and is still a very active research area by using experiments and atomic simulations (e.g., Trinkle *et al.*, 2003; Cerreta *et al.*, 2005; Ghosh *et al.*, 2014; Zong *et al.*, 2014a,b,c; Morrow *et al.* 2017a, b), and there are multiple possible pathways for the $\alpha \rightarrow \omega$ transformation (see examples in (Ghosh *et al.*, 2014)). When considering conditions of extreme mechanical loading at initial low temperature, the transformation from α phase HCP to ω phase hexagonal is the path of interest (Cerreta *et al.*, 2006a, b; Morrow *et al.*, 2017a, b; Young, 1976; Zong *et al.*, 2014b;). The materials Ti and Zr both produce meta-stable ω phase at high pressure, which is retained upon release (Cerreta *et al.*, 2006a, 2013; Morrow *et al.*, 2017a, b; Jones *et al.*, 2017). This also affords the opportunity to perform metallographic analysis on recovered samples which would not be possible otherwise. The structural phase transformation in these HCP materials affords interesting challenges to computational representation given prevalence of both dislocation slip as well as deformation twinning taking place during a single deformation history. MD calculations of rapidly loaded Ti have suggested that the pathway for the transformation process takes place following deformation twinning and is responsible for the observed orientation relationship between the untwinned and ω phase regions (Zong *et al.*, 2014b;) of the material. This work has also attempted to describe experimentally observed events. The phase transformation response of HCP materials has also received attention for static high pressure environments (Feng *et al.*, 2016; Feng and Levitas, 2017a, b, c; Levitas *et al.*, 2006). These materials offer the important opportunity to study the interaction of plasticity processes with those of structural phase transformation (Babaei and Levitas, 2018; Levitas and Preston, 2005; Levitas and Javanbakht, 2015; Levitas *et al.*, 2006). Recent work has suggested a possible interaction relationship such that dislocations are a potential mechanism for high pressure ω phase retention upon release (Low and Niezgoda, 2018).

The mechanics and physics communities have had a long presence in modeling of the structural evolution which takes place in materials with phase transformation (Abeyaratne and Knowles, 2006; Bhattacharya, 2004; Fujimoto, 2005; Gurtin, 1984, 1993; Khachaturyan, 2008). In doing so it is critical to develop and exercise theoretical frameworks that properly account for the thermodynamics of these strongly coupled processes. This is especially true for high

deformation rate conditions where energy levels are high and the dissipative actions of dislocation slip, deformation twinning, and transformation must be balanced together. Based upon both experimental and first principles calculation work, there has been important work done on Ti to develop a comprehensive empirical free energy potential for the finite elastic deformation and transformation processes (Greeff, 2001, 2004). This work was in particular focused on the pressure induced transformation from α to ω and based upon the functional form proposed in (Boettger and Wallace, 1997) for iron. This form of free energy employs three terms which account for the static lattice potential energy, lattice vibrational free energy, and electronic excitation free energy. Recently, there has been work to develop thermodynamically consistent frameworks for coupled plasticity and transformation processes which employ large deformation kinematic representations for application to large deformations at the macroscale (Adedoyin *et al.*, 2019; Feng *et al.*, 2017a, b, c) and at a single crystal level (Barton *et al.*, 2005; Feng *et al.*, 2018, 2019; Tjahjanto *et al.*, 2008; Turteltaub and Suiker, 2006) within continuum theories. The single crystal work is particularly important since the length scales of the physical interactions of dislocation slip, deformation twinning, and transformation are sub-granular and single crystal theories, which more readily accounts for the physics, can begin to be formulated—albeit still within a continuum setting. This also begins to afford the ability to address topics of grain size, grain boundaries and other microstructural features which continuum single crystal theories enable us to do with plasticity mechanisms alone.

Length scale effects and local structural evolution have been an important topic in plasticity work and there are many answered questions related to these effects on the interaction of plastic processes with high-pressure phase transformations during dynamic loading (Anand *et al.*, 2015; Hansen *et al.*, 2010; Tomellini and Politi, 2019). Here, we begin to address very simple questions of the effects of length scale and dimensionality on plasticity and transformation. The experimental results, which serve to guide and motivate the approach taken here, demonstrate significant structural evolution during dynamic loading conditions (Cerreta *et al.*, 2013, 2014; Morrow *et al.*, 2016, 2017a,b). In Cerreta *et al.*, (2013), four polycrystalline samples of Zr which were shock loaded at two different initial temperatures (25 °C and 200 °C) and two different impact velocities (nominally 650 m/s and 830 m/s), showed significant differences in the degree of structural evolution. Micro-hardness probing of the recovered samples, allowed for estimation of relative contributions from the mechanisms of dislocation

slip, deformation twinning, and $\alpha \rightarrow \omega$ phase transformation. The greatest quantitative impact upon micro-indentation resistance was assessed to come from both slip and transformation mechanisms with also measureable contributions from deformation twinning. The evolved microstructure as evidenced by recovered sample EBSD images for all four samples illustrated a transformation to a highly heterogeneous grain topology with little resemblance to the original microstructure. Further analysis of this material was presented by Morrow *et al.* (2017) where it was suggested that ω phase variant pathway is an important element in structural evolution and deformation twinning plays an important role, as well, but is poorly understood. Single crystal Ti was dynamically loaded using a Split-Hopkinson Pressure Bar (SHPB) system and examined in detail (Morrow *et al.*, 2016; Feng *et al.*, 2018). These results suggest that in addition to dislocation motion, twinning occurred in much of the material during deformation up to strains of 0.25. The deformed material structure was extremely dependent upon loading direction relative to the crystal orientation and found to be highly heterogeneous with very high dislocation density as evidenced by TEM micrographs. Although plate impact loading does not reach these high levels of plastic strain, the experiments demonstrate that structural evolution is substantial with corresponding changes in heterogeneity – from the basic length scale of the single crystal to the evolved length scales of dislocations/dislocation cells, and deformation twins. This correlates with shock loaded single crystal specimens which also contained ω phase regions. This work will take small steps to begin to address these complex three-dimensional structural evolution questions by staying close to the available experimental results.

In this paper, vectors and tensors are written as boldface and non-italic symbols. We define contractions of the second-order tensors $\mathbf{A} = \{A_{kl}\}$ and $\mathbf{B} = \{B_{mn}\}$ over one and two indices as $\mathbf{A} \cdot \mathbf{B} = \{A_{kl}B_{lm}\}$ and $\mathbf{A} : \mathbf{B} = \{A_{kl}B_{lk}\}$, respectively. Similarly, contractions of the forth-order tensor $\mathbf{K}$ and second-order tensor $\mathbf{A}$, over one and two indices are designated as $\mathbf{K} \cdot \mathbf{A} = \{K_{klmn}A_{ni}\}$ and $\mathbf{K} : \mathbf{A} = \{K_{klmn}A_{nm}\}$.

2. A complete system of equation and material parameters

Feng *et al.* (2018, 2019) formulated a thermodynamically consistent system of equations for single crystal titanium under plate impact loading, further developed the one-dimensional finite element model and numerically reproduced multiple experimental results such as the free

surface velocity, crystallographic texture, phase transformation pressures, and phase volume fractions. In this paper, we extend the model in Feng *et al.* (2018, 2019) into three dimensional models and also consider the grain boundary effects in bi-crystals on the plasticity and phase transformations. The constitutive equations in the single crystal theory presented by Feng *et al.* (2018, 2019) are used in this paper and are summarized as below.

2.1 Kinematics

The material motion is described by a continuous vector function $\mathbf{r} = \mathbf{r}(\mathbf{r}_0, t)$, where $\mathbf{r}$ and $\mathbf{r}_0$ are the position vectors of material points in the actual configuration Ω at the time instant t and in the reference configuration Ω_0 at the instant t_0 , respectively. The deformation gradient $\mathbf{F} = \frac{\partial \mathbf{r}}{\partial \mathbf{r}_0}$ can be multiplicatively decomposed into twinning $\mathbf{F}_{tw}$, phase transformation $\mathbf{F}_{pt}$, plastic slip $\mathbf{F}_{sl}$, and elastic $\mathbf{F}_e$ contributions:

$$\mathbf{F} = \mathbf{F}_e \cdot \mathbf{F}_{sl} \cdot \mathbf{F}_{pt} \cdot \mathbf{F}_{tw}. \quad (1)$$

In Eq. (1), plastic slip and twinning are considered separately, and they are separated by $\mathbf{F}_{pt}$. Since slip and twinning describe two different physical behaviors, it is reasonable to consider them in two configurations. The sequence for inelastic processes (Ω_{sl} , Ω_{pt} and Ω_{tw}) is chosen in Eq. (1) for two reasons. First, the plastic slip configuration Ω_{sl} follows from Ω_{pt} and Ω_{tw} because we consider plastic slip occurring in both the α twinned variants and the ω variants, and therefore plastic slip happens after the new α and ω variants are generated. Second, the configuration Ω_{pt} is chosen after Ω_{tw} because phase transformation in α twinned variants is considered and it occurs after the α variants are formed. Meanwhile, it is common to see other choices of the sequences among phase transformation, slip and twinning, and we admit that other choices are also admissible and may have their own advantages. Separating the four processes of elasticity, slip, twinning, and phase transformation into four different configurations as shown in Eq. (1) is beneficial to develop the driving force for each process by using the second law of thermodynamics.

The velocity gradient $\mathbf{L} = \dot{\mathbf{F}} \cdot \mathbf{F}^{-1}$ yields

$$\begin{aligned} \mathbf{L} = \dot{\mathbf{F}} \mathbf{F}^{-1} &= \dot{\mathbf{F}}_e \cdot \mathbf{F}_e^{-1} + \mathbf{F}_e \cdot \dot{\mathbf{F}}_{sl} \cdot \mathbf{F}_{sl}^{-1} \cdot \mathbf{F}_e^{-1} + \mathbf{F}_e \cdot \mathbf{F}_{sl} \cdot \dot{\mathbf{F}}_{pt} \cdot \mathbf{F}_{pt}^{-1} \cdot \mathbf{F}_{sl}^{-1} \cdot \mathbf{F}_e^{-1} \\ &+ \mathbf{F}_e \cdot \mathbf{F}_{sl} \cdot \mathbf{F}_{pt} \cdot \dot{\mathbf{F}}_{tw} \cdot \mathbf{F}_{tw}^{-1} \cdot \mathbf{F}_{pt}^{-1} \cdot \mathbf{F}_{sl}^{-1} \cdot \mathbf{F}_e^{-1} = \mathbf{L}_e + \mathbf{L}_{sl} + \mathbf{L}_{pt} + \mathbf{L}_{tw}. \end{aligned} \quad (2)$$

The Green-Lagrange elastic strain tensor $\mathbf{E}_e$ is

$$\mathbf{E}_e = \frac{1}{2} (\mathbf{F}_e^T \cdot \mathbf{F}_e - \mathbf{I}). \quad (3)$$

In this paper each variant of the HCP α and hexagonal ω phase is called as one “component”, and therefore each component not only distinguishes different phases but also distinguishes different variants within the same phase. The velocity gradient due to the dislocation slip is defined as

$$\mathbf{L}_{sl} = \dot{\mathbf{F}}_{sl} \cdot \mathbf{F}_{sl}^{-1} = \sum_i \sum_{\beta} c_i \dot{\gamma}_{\beta i - sl} \mathbf{s}_{\beta i} \otimes \mathbf{m}_{\beta i}, \quad \dot{\gamma}_{\beta i - sl} = \rho_{M\beta i} b_{\beta i} v_{\beta i}. \quad (4)$$

The slip rate $\dot{\gamma}_{\beta i - sl}$ is from the slip system β of the i -th component. In this paper, the subscripts i and j refer to the different components, and β and η refer to different slip systems. For the α phase, there are 12 pyramidal slip systems and 3 prismatic slip systems considered. For the ω phase of Ti, there are 3 basal slip and 3 prismatic systems considered. The detail of slip orientations for slip system can be found in Feng *et al.* (2019). Single crystal α phase may form six possible compression twin variants when compressed along the c -axis of the lattice (Feng *et al.*, 2018, 2019). These six α phase twin variants plus initial parent material may further transform into seven ω phase variants under high pressure (Feng *et al.*, 2019). The summation over index i in Eq. (4) is from $i=0$ to $i=13$, in which $i=0$ represents the parent α material, $i=1$ to 6 are for six twin variants. For the ω phase, i varies from 7 to 13, and the summation of β is from 1 to 6 for six slip systems. For each α variant, the summation of β is from 1 to 15 for fifteen slip systems. In Eq. (4), Burgers vector is $b_{\beta i}$, c_i is the mass fraction or the volume fraction of the i -th phase component, vector $\mathbf{s}_{\beta i}$ is the slip direction, $\mathbf{m}_{\beta i}$ represents the slip plane normal, and mobile dislocation density is $\rho_{M\beta i}$ with a mean velocity $v_{\beta i}$.

The velocity gradient due to deformation twinning is designated as

$$\mathbf{L}_{tw} = \dot{\mathbf{F}}_{tw} \cdot \mathbf{F}_{tw}^{-1} = \sum_i \dot{\gamma}_{i-tw} \mathbf{b}_i \otimes \mathbf{n}_i, \quad (8)$$

where the material parameter γ_w is a shear strain magnitude caused by deformation twinning when the parent material fully transforms into one of the six possible α twin variants, the vector $\mathbf{b}_i$ represents the twinning direction and $\mathbf{n}_i$ stands for the twinning plane normal for the i -th compressive twin. For six compressive twins (i.e. primary twins), the summation of i is from 1 to 6. At any instant t , the concentration rate of the i -th compressive twin $\dot{\mathcal{C}}_i$ can be decomposed into two contributions: $\dot{\mathcal{C}}_i = \dot{\mathcal{C}}_{i-tw} + \dot{\mathcal{C}}_{i-pt}$, in which nonnegative $\dot{\mathcal{C}}_{i-tw}$ is due to the parent α component twinned into the i -th twin and non-positive $\dot{\mathcal{C}}_{i-pt}$ is caused by phase transformation from the i -th twin to ω phase. When the parent material transforms to the compressive twin phases, we have $\dot{\mathcal{C}}_{0-tw} = -\sum_{i=1}^6 \dot{\mathcal{C}}_{i-tw}$, and when the α phase transforms to the ω phase, it yields $\dot{\mathcal{C}}_{i-pt} \big|_{i=0 \text{ to } 6} = -\dot{\mathcal{C}}_{j-pt} \big|_{j=i+7}$.

Transformational deformation gradient and its rate are defined as

$$\mathbf{F}_{pt} = \mathbf{I} + \sum_{i=7}^{13} c_i \boldsymbol{\varepsilon}_{i-pt}, \quad \dot{\mathbf{F}}_{pt} = \sum_{i=7}^{13} \dot{\mathcal{C}}_i \boldsymbol{\varepsilon}_{i-pt}. \quad (9)$$

In Eq. (9), the strain tensor $\boldsymbol{\varepsilon}_{i-pt}$ determines the transformational deformation of materials when the i -th ($i = j-7$) α component completely transforms into the j -th ω component. The quantity $\dot{\mathcal{C}}_i$ (or c_i) for the ω components in Eq. (9) is equal to or greater than zero because further transformation from the ω phase to other phases such as β phase only occurs at much higher temperature or pressure than the experiments and simulations considered in this study.

2.2 Nonlinear elasticity model

For small elastic deformation, the Helmholtz free energy can be defined as

$$\Psi = \sum_{i=0}^{13} c_i \left(\frac{1}{2} \mathbf{E}_e : \mathbf{C}_i : \mathbf{E}_e \right), \quad (10)$$

where $\mathbf{C}_i$ is the fourth-order elastic stiffness tensor of the i -th component.

Further, Cauchy stress $\boldsymbol{\sigma}$ and the second Piola-Kirchhoff stress $\mathbf{T}$ is given as,

$$\boldsymbol{\sigma} = \frac{1}{\det \mathbf{F}_e} \mathbf{F}_e \cdot \frac{\partial \Psi}{\partial \mathbf{E}_e} \cdot \mathbf{F}_e^T = \frac{1}{\det \mathbf{F}_e} \mathbf{F}_e \cdot \sum_{i=0}^{13} c_i (\mathbf{C}_i : \mathbf{E}_e) \cdot \mathbf{F}_e^T = \frac{1}{\det \mathbf{F}_e} \mathbf{F}_e \cdot \sum_{i=0}^{13} c_i \mathbf{T}_i \cdot \mathbf{F}_e^T. \quad (11)$$

For high pressure problems, the volumetric part of the Cauchy stress, i.e. pressure, may increase up to a large value, becoming very nonlinear function of the volumetric strain. The pressure p_{eos} obtained from the nonlinear equation of state (EOS) in Greeff *et al.* (2001) has an excellent correspondence with experiments for Ti for pressures up to 80 GPa. The EOS has been constructed by developing a parametrized Helmholtz free energy as a function of temperature θ and specific volume v (volume per unit mass) in the current configuration Ω ,

$$\psi_{eos} = \psi_0(v) + \psi_{el}(v, \theta) + \psi_{vib}(v, \theta), \quad (12)$$

in which $\psi_0(v)$, $\psi_{el}(v, \theta)$, and $\psi_{vib}(v, \theta)$ stand for the static lattice potential, electronic excitation energy, and ion motion free energies, respectively. Their analytical expressions in Greeff *et al.* (2001) are as follows:

$$\psi_0(v) = \psi^* + \frac{4v^* B^*}{(B_1^* - 1)^2} [1 - (1 + \eta) e^{-\eta}]; \quad \eta = \frac{3}{2} \left[\left(\frac{v}{v^*} \right)^{1/3} - 1 \right] (B_1^* - 1). \quad (13)$$

$$\psi_{el}(v, \theta) = -\frac{1}{2} \Gamma_0 \left(\frac{v}{v_0} \right)^\kappa \theta^2. \quad (14)$$

$$\psi_{vib}(v, \theta) = 2R\theta \left[\frac{1}{40} \left(\frac{\theta_2(v)}{\theta} \right)^2 - \ln \left(\frac{\theta}{\theta_0(v)} \right) \right], \quad \left(\theta_0(v) = \theta_0^* e^{\frac{\gamma_0}{v_0}(v-v_0)}; \theta_2(v) = \theta_0(v) e^{1/3} \right). \quad (15)$$

In Eqs. (13)-(15), v^* represents the equilibrium volume, B^* and B_1^* are the bulk modulus and its pressure derivative respectively, ψ^* controls the relative free energy of the two phases, v_0 is the specific volume at zero pressure, θ_0^* is the moment of the phonon spectrum. R, Γ_0, κ , and γ_0 in Eqs. (13)-(15) are also material parameters given in Greeff *et al.* (2001). It is noted that this form of the Helmholtz free energy does not employ the entire stress tensor but only the volumetric term. The Cauchy stress with EOS pressure representation for homogeneous single-phase materials is given by

$$\boldsymbol{\sigma} = \left(\frac{1}{\det \mathbf{F}_e} \cdot \mathbf{F}_e \cdot (\mathbf{C} : \mathbf{E}_e) \cdot \mathbf{F}_e^t \right)_{dev} - p_{eos} \mathbf{I}, \quad \left(p_{eos} = -\frac{\partial \psi_{eos}}{\partial v} \right). \quad (16)$$

For heterogeneous materials with the combined α and ω system, the pressure can be expressed as

$$p_{eos} = \sum_{i=0}^6 c_i p_{eos-\alpha} + \sum_{i=7}^{13} c_i p_{eos-\omega}, \quad (17)$$

where $p_{eos-\alpha}$ and $p_{eos-\omega}$ is the pressure from the EOS by using Eqs. (12) - (16) for the α and ω phases by assuming a constant deformation gradient within each of the phases.

2.3 Deformation twinning and phase transformation

Salem *et al.* (2005) studied deformation twinning in single crystal HCP Ti, where the rate of twinning in Ti is determined by a power law of the resolved shear stress. Based on the theory in Salem *et al.* (2005), Feng *et al.* (2019) developed the thermodynamic driving force for the $(\mathbf{b}_i, \mathbf{n}_i)$ twin system expressed as $\tau_{i-tw} = \mathbf{F}_{pt}^{-1} \cdot \mathbf{F}_{sl}^{-1} \cdot \mathbf{F}_e^{-1} \cdot \boldsymbol{\sigma} \cdot \mathbf{F}_e \cdot \mathbf{F}_{sl} \cdot \mathbf{F}_{pt} : (\mathbf{b}_i \otimes \mathbf{n}_i)$. The evolution of twin volume fraction is defined as,

$$\dot{c}_{i-tw} \Big|_{i=1,2,\dots,6} = \begin{cases} 0 & \text{if } \tau_{tw-i} < \tau_{tw0} \\ \left(1 - \sum_{j=7}^{13} c_j \right) (1 - c_i^{b_0}) \frac{\dot{\gamma}_0}{\gamma_{tw}} \left(\frac{\tau_{tw-i}}{S_{tw}} \right)^{d_0} & \text{if } \tau_{tw-i} \geq \tau_{tw0} \end{cases}. \quad (18)$$

where the material parameter $\dot{\gamma}_0$ is the reference shear strain rate, and the reference shear stress S_{tw} with the initial value S_{tw0} and evolves by

$$\dot{S}_{tw} = h_{sl} \left(\sum_j \sum_\beta c_j \dot{\gamma}_{\beta j-sl} \right) \left(\sum_j \sum_\beta c_j \gamma_{\beta j-sl} \right)^{g_0} + h_{tw} \left(\sum_i \gamma_{tw} \dot{c}_i \right) \left(\sum_i c_i \right)^{e_0}. \quad (19)$$

Here, $\sum_j \sum_\beta c_j \gamma_{\beta j-sl}$ represents the total shear strain due to plastic slip of both untwinned and

twinning regions; $\left(\sum_i \gamma_{tw} \dot{c}_i \right)$ stands for the equivalent shear rate of the i -th twin system;

h_{tw} , e_0 , h_{sl} and g_0 are material parameters. Experimental observations show (Cerreto *et al.*, 2005, 2006a, b, 2010, 2013) that twinning is observed to occur within the α phase but has not

been observed within the ω phase. Therefore, in this model we consider deformation twinning only within the α phase.

Both atomistic simulation (Zong *et al.*, 2014, 2016) and experiment (Morrow *et al.*, 2016, 2017a, b) under high strain rate loading suggests that phase transformation is prominent within only the twinned regions of the α phase and this twinning is responsible for a large rotation between the α and ω phases orientation relationship. Therefore, the pathway through twinning before the α to ω phase transition remains a hypothesis which is applied here.

As we developed in Feng *et al.* (2018), the driving force for phase transformation is

$$X_{i-pt} \approx \mathbf{F}_{pt}^{-1} \cdot \mathbf{F}_{sl}^{-1} \cdot \mathbf{F}_e^{-1} \cdot \boldsymbol{\sigma} \cdot \mathbf{F}_e \cdot \mathbf{F}_{sl} : \boldsymbol{\varepsilon}_{i-pt} - \rho(\psi_{eos-\omega} - \psi_{eos-\alpha}). \quad (20)$$

An exponential law suggested in Greeff *et al.* (2001) for rate of change of phase volume fraction is utilized as follows:

$$\dot{X}_{i-pt} = \left[1 - (c_{i-pt})^{p_1} \right] w \frac{X_{i-pt}}{\beta_{tr}} \exp \left\{ \left(\frac{X_{i-pt}}{\beta_{tr}} \right)^{q_1} \right\}, \quad (21)$$

in which w and β_{tr} are the kinetic parameters that control phase transformation rate.

2.4 Dislocation-based crystal plasticity model

Hansen *et al.* (2013) formulate an advanced dislocation-based constitutive model for the deformation of metallic single crystals over a wide range of strain rates including shock compression loading considered in this paper. Moreover, the different types of dislocation density and their evolution and interaction is considered in Hansen *et al.* (2013), and we may trace the dislocation density variations during the loading. By modifying their theory to include plastic slip in different variants and phases, Feng *et al.* (2019) developed a thermodynamically consistent dislocation-based viscoplasticity model for multicomponent heterogeneous materials. The slip rate $\dot{\gamma}_{\beta i}$ for a specific slip system, and total slip rate $\dot{\mathbf{F}}_{sl} \cdot \mathbf{F}_{sl}^{-1}$ for all slip systems can be defined as

$$\dot{\gamma}_{\beta i} = b_{\beta i} \rho_{M\beta i} v_{\beta i}; \quad \mathbf{L}_{sl} = \dot{\mathbf{F}}_{sl} \cdot \mathbf{F}_{sl}^{-1} = \sum_i \sum_{\beta} c_i \dot{\gamma}_{\beta i} (\mathbf{s}_{\alpha i} \otimes \mathbf{m}_{\alpha i}). \quad (22)$$

Here, $v_{\beta i}$ is the average dislocation velocity on the slip system β , and $\rho_{M\beta i}$ is the corresponding mobile dislocation density inside the i -th component. The real mobile dislocation density is

averaged over a representative volume as $N_{M\eta_i} = c_i \rho_{M\beta}$, where $N_{M\eta_i}$ is the volume fraction of the i -th component. We only consider the statistically stored dislocation density and ignore geometrically necessary dislocations as a first description of this complex physical process. The velocity $v_{\beta i}$ determines the sign of $\frac{\tau_{\beta i}}{B_{\beta i}}$, and it can be written as (Luscher *et al.*, 2017)

$$v_{\beta i} = \frac{\tau_{\beta i} b_{\beta i}}{B_{\beta i}}, \quad B_{\beta i} = \frac{B_0}{1 - (v_{\beta i} / c_s)^2}, \quad (23)$$

where $B_{\beta i}$ is the viscous drag coefficient for slip system β of the i -th component; $b_{\beta i}$ is the magnitude of the Burgers vector; B_0 is the drag coefficient at zero velocity $v_{\beta i} = 0$; c_s is the shear wave speed. The resolved shear stress $\tau_{\beta i} = \mathbf{F}_e^{-1} \cdot \boldsymbol{\sigma} \cdot \mathbf{F}_e : (\mathbf{s}_{\beta i} \otimes \mathbf{m}_{\beta i})$ is the only term determining the sign of $v_{\beta i}$ as positive, negative or zero.

We assume that dislocations fall into three classes of populations in this paper as in Hansen *et al.* (2013) and Feng *et al.* (2018, 2019): (1) mobile dislocations (subscript M) is the only population having nonzero velocity in a material, (2) pileup dislocations (subscript P) generated during pileup of mobile dislocations and are able to become mobile again if they escape from the temporary sessile state, and (3) locked sessile dislocations (subscript L) do not belong to any slip system and are generated when the mobile dislocations form locks and become sessile.

The change rate $\dot{N}_{A\eta_i-B\beta j}^{inter}$ of dislocation density $N_{A\eta_i}$ - the i -th component for type A on slip system η by the interaction with $N_{B\beta j}$ can be defined as

$$\dot{N}_{A\eta_i-B\beta j}^{inter} = P_{A\eta_i-B\beta j}^{inter} D_{A\eta_i-B\beta j}^{inter} f_{A\eta_i-B\beta j}^{inter} N_{A\eta_i} N_{B\beta j} |\mathbf{v}_{A\eta_i-B\beta j}|. \quad (24)$$

This rate $\dot{N}_{A\eta_i-B\beta j}^{inter}$ indicates that the dislocation density $N_{A\eta_i}$ changes from one type into another type (i.e. from P to M , from M to L , from M to P , etc.). $D_{A\eta_i-B\beta j}^{inter}$ is the distance within which the interactions between $N_{A\eta_i}$ and $N_{B\beta j}$ can take place. $|\mathbf{v}_{A\eta_i-B\beta j}|$ is the absolute value of the relative velocity of dislocations between these two slip systems. $f_{A\eta_i-B\beta j}^{inter}$ is the fraction of dislocation density $N_{A\alpha i}$ that interacts with $N_{B\beta j}$. The thermal probability $P_{A\alpha i}^{inter}$ is introduced as the thermal

barrier for the occurrence of an interaction, and the details can be further seen in Hansen *et al.* (2013) and Feng *et al.* (2019).

For an effective interaction between two slip systems, at least one of the two slip systems must be mobile to have a nonzero relative velocity $|\mathbf{v}_{A\eta i-B\beta j}|$ in Eq. (24). There are three types of interactions between mobile dislocations $N_{M\eta i}$, when they meet with the slip system $N_{B\beta j}$ and cause reduction of the population $N_{M\eta i}$. Firstly, mobile dislocations $N_{M\eta i}$ pile up ($\dot{N}_{M\eta i-B\beta j}^{pile-M\eta i}$) and become pileup dislocations; secondly, they annihilate ($\dot{N}_{M\eta i-B\beta j}^{anni-M\eta i}$) and reduce the total line density; thirdly, they can form sessile locks ($\dot{N}_{M\eta i-B\beta j}^{lock-M\eta i}$) and become sessile dislocations:

$$\dot{N}_{M\eta i}^{inter} = \sum_B \sum_{\beta} \sum_j \dot{N}_{M\eta i-B\beta j}^{inter} = \sum_B \sum_{\beta} \sum_j \dot{N}_{M\eta i-B\beta j}^{pile-Mai} + \sum_B \sum_{\beta} \sum_j \dot{N}_{M\eta i-B\beta j}^{lock-Mai} + \sum_B \sum_{\beta} \sum_j \dot{N}_{M\eta i-B\beta j}^{anni-Mai}. \quad (25)$$

Here, $\dot{N}_{M\eta i}^{inter}$ represents the total change rate of mobile dislocation density $N_{M\eta i}$ during interactions with all other dislocations.

Since $N_{A\eta i} = c_i \rho_{A\eta i}$, and assuming that $\dot{\epsilon} = 0$ during plastic slip, we obtain

$$\dot{N}_{A\eta i}^{inter} = \dot{\epsilon} \rho_{A\eta i}^{inter} + c_i \dot{\rho}_{A\eta i}^{inter} = c_i \dot{\rho}_{A\eta i}^{inter}, \quad (26)$$

Further, we have

$$\dot{\rho}_{A\eta i}^{inter} = \sum_B \sum_{\beta} \sum_j P_{A\eta i-B\beta j}^{inter} D_{A\eta i-B\beta j}^{inter} f_{A\eta i-B\beta j}^{inter} \rho_{A\eta i} N_{B\beta j} |\mathbf{v}_{A\eta i-B\beta j}|, \quad (27)$$

$$\dot{\rho}_{M\eta i}^{inter} = \sum_B \sum_{\beta} \sum_j \dot{\rho}_{M\eta i-B\beta j}^{lock} + \sum_B \sum_{\beta} \sum_j \dot{\rho}_{M\eta i-B\beta j}^{pile-Mai} + \sum_B \sum_{\beta} \sum_j \dot{\rho}_{M\eta i-B\beta j}^{anni-Mai}. \quad (28)$$

When mobile dislocation density $N_{M\eta i}$ interacts with others, it causes dislocation density population reduction. However, there are several sources that can cause its increase: (1) homogeneous nucleation $\dot{\rho}_{M\eta i}^{gen}$, (2) mobile dislocation propagation $\dot{\rho}_{M\eta i}^{prop}$, and (3) escape of pileup dislocations $\dot{\rho}_{M\eta i}^{esc}$. The total mobile dislocation density in the slip system η of the i -th phase yields:

$$\dot{\rho}_{M\eta i} = \dot{\rho}_{M\eta i}^{gen} + \dot{\rho}_{M\eta i}^{prop} + \dot{\rho}_{M\eta i}^{esc} - \dot{\rho}_{M\eta i}^{inter}. \quad (29)$$

The homogeneous nucleation of dislocations $\rho_{M\eta i}^{en}$ occurs within a perfect lattice, which requires large thermal fluctuations or large external stress and as such it is ignored as Hansen *et al.* (2013) and Luscher *et al.* (2017). The mobile dislocation propagation $\rho_{M\eta i}^{prop}$ can be written as

$$\rho_{M\eta i}^{prop} = k_{\eta i} \rho_{M\eta i} |v_{\eta i}| / \bar{r}_{M\eta i}, \quad (30)$$

in which the material parameter $k_{\eta i}$ is the propagation coefficient and $\bar{r}_{M\eta i}$ is the average mobile dislocation loop radius of curvature.

There are two physical sources causing the escape of pileup dislocations $\rho_{P\eta i}^{esc}$. One is the thermal escape of pileup dislocations $\rho_{P\eta i}^{esc\theta}$ due to thermal fluctuation with assistance from external stresses:

$$\rho_{P\eta i}^{esc\theta} = \frac{1}{t_{P\eta i}^{esc\theta}} P_{P\eta i}^{esc}, \quad (31)$$

in which $t_{P\eta i}^{esc\theta}$ is the time constant equal to the average time of a thermal fluctuation. The other source $\sum_{\beta} \sum_j \rho_{P\eta i-M\beta j}^{esc-inter}$ is caused by pileup dislocation that escape via interaction with the mobile dislocations based on Eq. (25).

Pileup dislocations are generated due to the pileup of mobile dislocations on obstacles, and reduced due to escape, annihilation, and lock formation. The evolution of pileup dislocations is written as

$$\dot{\rho}_{P\eta i} = \sum_B \sum_{\beta} \sum_j \rho_{M\eta i-B\beta j}^{pile-Mai} - \rho_{P\eta i}^{escT} - \sum_{\beta} \sum_j \rho_{P\eta i-M\beta j}^{esc-inter} - \rho_{M\eta i-P\eta i}^{anni-MP} - \sum_{\beta} \sum_j \rho_{P\eta i-M\beta j}^{lock-inter}. \quad (32)$$

The locked dislocation density is created as the mobile dislocations interact with the pileup or mobile dislocations to leave sessile locked debris in a material

$$\dot{N}_{M\eta i}^{lock} = \sum_{M\eta i} \sum_{B\beta j} N_{M\alpha i-B\beta j}^{lock} = \sum_{M\eta i} \sum_{B\beta j} P_{M\eta i-B\beta j}^{lock} D_{M\eta i-B\beta j}^{lock} f_{M\eta i-B\beta j}^{lock} N_{M\eta i} N_{B\beta j} |v_{A\eta i-B\beta j}|. \quad (33)$$

2.5 Evolution of temperature

The change of temperature is calculated by the total dissipation energy converted into thermal energy and stored in a material. Based on the second law of thermodynamics, the temperature variation follows:

$$\theta = \frac{1}{\rho c_v} \left(k_1 \sum_i \sum_\beta c_i \tau_{\beta i} \dot{\theta}_{sl-\beta i} + k_2 \sum_j \tau_{j-tw} \dot{\theta}_{tw} + k_3 \sum_m X_{m-pt} \dot{\theta}_{m-pt} \right). \quad (34)$$

Here, the specific heat at constant volume is defined: $c_v = -\theta \frac{\partial^2 \psi}{\partial \theta^2}$; k_1 , k_2 and k_3 are the ratios of dissipative energy due to plastic slip, twinning, and phase transformation respectively stored as the thermal energy in the material. From Morrow *et al.* (2017a, b), the time for shockwave transmission from the impact plane to free surface plane is less than 0.5 μs . Therefore, we assume adiabatic conditions here. More details on the non-equilibrium thermodynamics of dislocation slip processes are discussed in Lieou *et al.* (2018, 2019).

3. Experiment and one-dimensional model for plate impact experiment

It has been demonstrated that plate impact experiment under uniaxial strain loading can be valuable for investigating mechanical behaviors of materials at high strain rates. A high-purity Ti multi-crystal sample composed of four large grains, each extending through the specimen thickness, was investigated experimentally via plate impact in Morrow *et al.* (2017b). As shown in Fig. 1, each grain represented a different crystal orientation relative to the impact load direction which points out of the plane. The diameter and thickness of Ti sample in Fig. 1 are 10.06 mm and 1.502 mm, and it was embedded in a standard polycrystalline Ti momentum trap ring assembly. The thickness and diameter of the polycrystalline copper flyer was 2.032 mm and 38 mm. A photon Doppler velocimetry (PDV) probe aligned to measure the free surface velocity, opposite the impact plane.

In Feng *et al.* (2019), this experiment was mimicked in simulation. To discover the possible physics occurring in the crystals under high strain rate, two shocked crystals of $[0001]$ and $[10\bar{1}1]$ orientations, from the sample in Fig. 1, are investigated in this paper. The material parameters for the processes of nonlinear elasticity, plastic slip, mechanical twinning, and phase transformations are used directly from Feng *et al.* (2019).

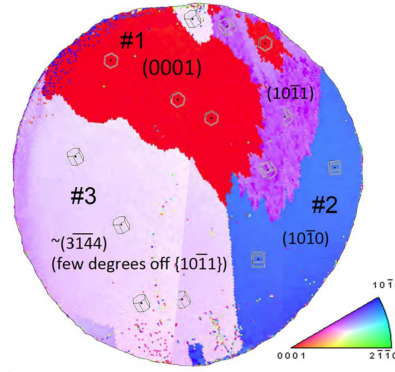


Fig. 1. Ti multi-crystal sample and the source of the experimental results adopted from Morrow *et al.* (2017b).

4. Finite element model and results for plate impact experiment

In Feng *et al.* (2019), the simulation of uniaxial strain loading in $[0001]$ and $[10\bar{1}1]$ direction uniaxial strain loading was investigated with one-dimensional simulations. In that analysis, the copper flyer is not directly represented, but a constant velocity 600 m/s boundary conditions is applied at the impact plane. In section 4.1, a one-dimensional model with an explicit copper flyer is considered, which will examine the feasibility of application of the constant velocity in Feng *et al.* (2019). In section 4.2, three-dimensional plate impact models will be considered and anisotropy in the x and y directions will be discussed. In section 4.3, the bicrystal with grain boundary interface will be examined, and results will be compared with those of the single crystal model alone. For both one-dimensional and three-dimensional simulations, the maximum time increment step is chosen as 1.5×10^{-10} s while total loading time is around 5×10^{-7} s. Our simulations are not time-increment-step dependent because we obtained the same results after reducing the time increment step to 0.75×10^{-10} s.

4.1 One-dimensional model for single crystals with the copper flyer

In Feng *et al.* (2019), single crystals of $[0001]$ and $[10\bar{1}1]$ under shock loading was studied with an assumption that the constant velocity as 600 m/s is applied at the impact plane, which means that the copper flyer is represented only implicitly. In this section, shock loading

along the $[0001]$ and $[10\bar{1}1]$ crystallographic directions will be investigated, with the copper flyer explicitly represented.

The linear relation between the shock velocity, U_s , and the particle velocity, U_p is given by

$$U_s = c_0 + sU_p. \quad (35)$$

The linear $U_s - U_p$ Hugoniot form can be written as

$$p = \frac{\rho_0 c_0^2 \eta}{(1 - s\eta)^2} \left(1 - \frac{\Gamma_0 \eta}{2} \right) + \Gamma_0 \rho_0 E_m. \quad (36)$$

E_m is the hydrostatic internal energy per unit mass ignoring elastic energy, and $\eta = 1 - \rho_0/\rho$ is the nominal volumetric compressive strain. Since shear deformation is small in copper under the loading considered in this paper, a linear relation between shear strain and stress is assumed. The elastic constants in Eqs. (35) and (36) are: $c_0 = 3940$ m/s, $s = 1.489$, $\rho_0 = 8941 \text{ kg/m}^3$ and $\Gamma_0 = 2.02$, and shear modulus is 47.7 GPa (Steinberg, 1996). For plastic deformation, the J_2 flow rule is used (Feng *et al.*, 2016),

$$\dot{\mathbf{\epsilon}}_p = \lambda \frac{\mathbf{s}}{\sqrt{\mathbf{s}:\mathbf{s}}} \quad (37)$$

Where $\dot{\mathbf{\epsilon}}_p$ is plastic strain tensor, $\mathbf{s}$ is the deviator of Cauchy stress, and λ is a scalar function (unit as 1/s), which is determined from the consistency condition $\dot{\phi} = 0$. Here ϕ is the plastic potential

$$\phi = \sqrt{3/2} \mathbf{s}:\mathbf{s} - \sigma_y = 0, \quad (38)$$

where σ_y is the yield strength of copper. The Johnson-Cook strength model is used for yield strength σ_y (Johnson and Holmquist, 1989)

$$\sigma_y = (A + B \epsilon_p^n) (1 + C \ln \dot{\epsilon}^*) (1 - T^{*m}), \quad (39)$$

in which ϵ_p is the equivalent plastic strain determined from $\dot{\epsilon}_p = \sqrt{2/3} \dot{\mathbf{\epsilon}}_p : \dot{\mathbf{\epsilon}}_p$; $\dot{\epsilon}^*$ is dimensionless plastic strain rate: $\dot{\epsilon}^* = \dot{\epsilon}_p / \dot{\epsilon}_0$ with $\dot{\epsilon}_0 = 1.0 \text{ s}^{-1}$; and homologous temperature $T^* = (T - T_{room}) / (T_{melt} - T_{room})$. In this paper, we only consider the variation of temperature in the Ti sample as in Feng *et al.* (2019), and ignore the temperature variation in the copper flyer. The

material constants in Eq. (39) are: $A = 89.6 \text{ MPa}$, $B = 291 \text{ MPa}$, $C = 0$, and $n = 0.31$ (Johnson and Holmquist, 1989). When the copper flyer is considered explicitly in the simulation, the impact plane velocity is almost the same for $[0001]$ and $[10\bar{1}1]$ single crystals, and rapidly increases from zero to a stable value around 580 m/s for $0.44 \mu\text{s}$ in Fig. 2. At $t = 0.44 \mu\text{s}$, the impact plane velocity begins to again increase rapidly. Fig. 3 plots the free surface velocity, and shows that the shockwave reaches the free surface at $t = 0.22 \mu\text{s}$ for both $[0001]$ and $[10\bar{1}1]$ single crystals. Consequently, it takes $0.44 = 0.22 \times 2 \mu\text{s}$ for the shockwave traveling from the impact plane to free surface, and then back to impact plane, which is the reason for the increased impact plane velocity at $t = 0.44 \mu\text{s}$. The thickness of the polycrystalline copper flyer and Ti sample is 2.032 mm and 1.502 mm , respectively, and at the time $t = 0.44 \mu\text{s}$ the reflected wave of copper flyer has not yet reached the impact surface.

Having almost the same impact plane velocity, the free surface velocity is very distinct between the $[0001]$ and $[10\bar{1}1]$ single crystals. In Fig. 3a for the $[0001]$ crystal, when the free surface velocity reaches 300 m/s , a plateau in velocity is found in both experiment and simulation, which is caused by twinning initiation. After this plateau and for the free surface velocity between 300 to 1000 m/s , the velocity slope is slightly smaller than the elastic front because dissipative twinning and plastic slip occur. At a free surface velocity of 1000 m/s in Fig. 3a, phase transformation appears, which leads to a significant reduction of slope in the free surface velocity curve in the simulation results. Afterwards, the free surface velocity becomes a constant at around 1100 m/s in both simulation and experiment. In Fig. 3a for the $[10\bar{1}1]$ crystal, the free surface velocity from both simulation and experiment shows good correspondence. At a velocity around 900 m/s , a significant reduction in the slope occurs, which is caused by both twinning and slip processes in the simulation, and the final stable velocity is realized at around 1120 m/s in simulation and experiment. Fig. 4 shows the von Mises stress and pressure along the copper the flyer thickness. The maximum pressure in the copper flyer is around 15 GPa , which is slightly higher than for Ti single crystals shown later in Figs. 9 and 15. However, the von Mises stress in the copper flyer is much smaller than the Ti single crystals, because polycrystal copper allows the plastic deformation in every direction but HCP single crystal slip is geometrically restricted.

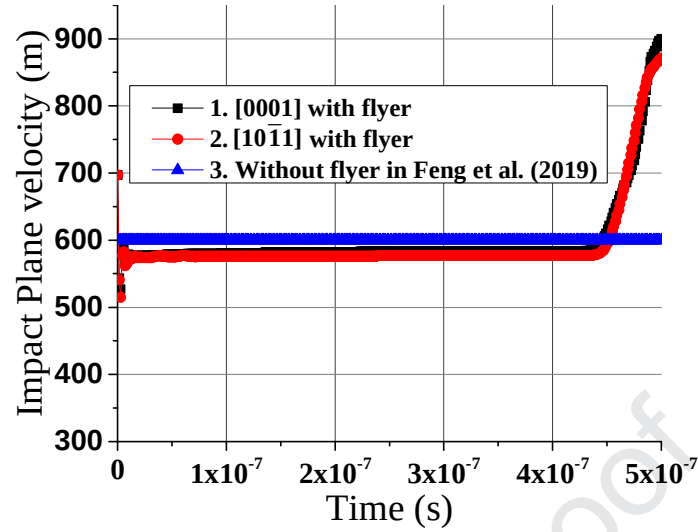


Fig. 2. Particle velocity at the impact plane between the single crystal Ti sample and the copper flyer for the 1D model. Curves 1 and 2 are for impact loading along the $[0001]$ and $[10\bar{1}1]$ direction of the single crystal, respectively. Curve 3 is for the constant velocity loading at 600 m/s applied to the impact plane.

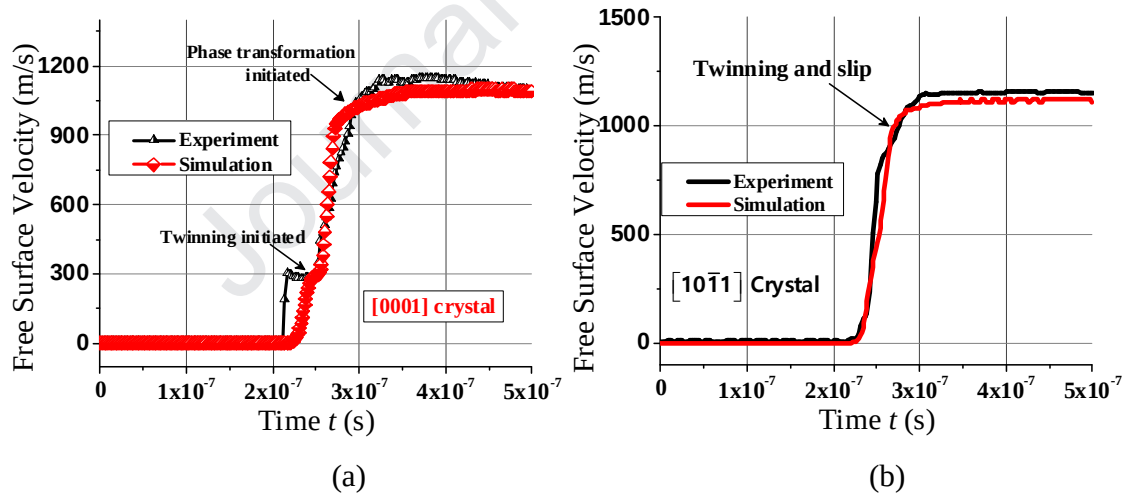


Fig. 3. Free surface velocity for single crystal Ti sample and the copper flyer for 1D model compared to the free surface velocity in experiments along the (a) $[0001]$ and (b) $[10\bar{1}1]$ crystallographic directions of loading. The arrows indicate events taking place within the simulations.

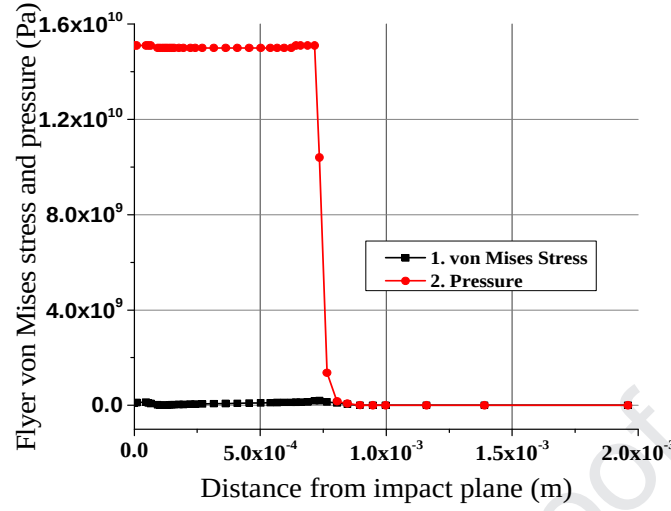


Fig. 4. von Mises stress and pressure for the copper flyer $t = 0.181\mu\text{s}$ as a function of the distance from the impact plane.

4.2 Three-dimensional model for single crystals with the copper flyer

In this section, three-dimensional models will be discussed, in which a cylindrical shape will be represented in both a Ti sample and Cu flyer. As Fig. 5 illustrates, we consider geometries where cylindrical systems with $10\ \mu\text{m}$ and $20\ \mu\text{m}$ radii are considered so that relative dimensions of the one and three-dimensional problems are considered. In addition, a polycrystal Ti momentum trap is used (Morrow *et al.*, 2017b) for the experiments, therefore the surface of the sample except for the free surface and impact plane has zero displacement in the x and y direction for all nodes on the cylinder surface, relative to the coordinate system given in Fig. 5. Similar simulations were used in the past to study the plate impact response of materials where complete spatial resolution of the problem was impossible (Becker, 2004, 2017; Becker and Callaghan 2018). In this section, we will discuss the effects of the sample radius and loading directions. In Section 4.2.1, the results for the $[0001]$ crystal are presented, while the $[10\bar{1}1]$ crystal is discussed in Section 4.2.2.

4.2.1 The $[0001]$ crystal

In this section, the $[0001]$ direction single crystal loading is investigated. The mesh of each of the two sample models and the Cartesian coordinate system used can be seen in Fig. 5. The z direction is along the shock direction and perpendicular to the impact plane which is at the right end of the model images in Fig. 5. The time instant $t = 0.181\mu\text{s}$ is chosen to display the

state variable fields of stress and the volume fraction of components such as parent material, alpha and omega variants. Fig. 5(a, c) shows that for both small and large samples, the pressure heterogeneity along the x and y directions are not large enough to display graphically. To see the inside of the numerical sample at loading, the sample mid-section between the free surface and impact plane is displayed in Fig 5 (b, d). Fig. 5(b, d) shows that at the mid-section of the sample, the pressure is also very homogeneous in the x and y directions, and the maximum pressure is located at the impact plane due to boundary effects. The high pressure around 15 GPa at the impact surface as shown in Fig. 4 causes the impact plane to have a slightly higher pressure than the rest of the sample, and there is some heterogeneity in pressure in the region very close to the impact surface.

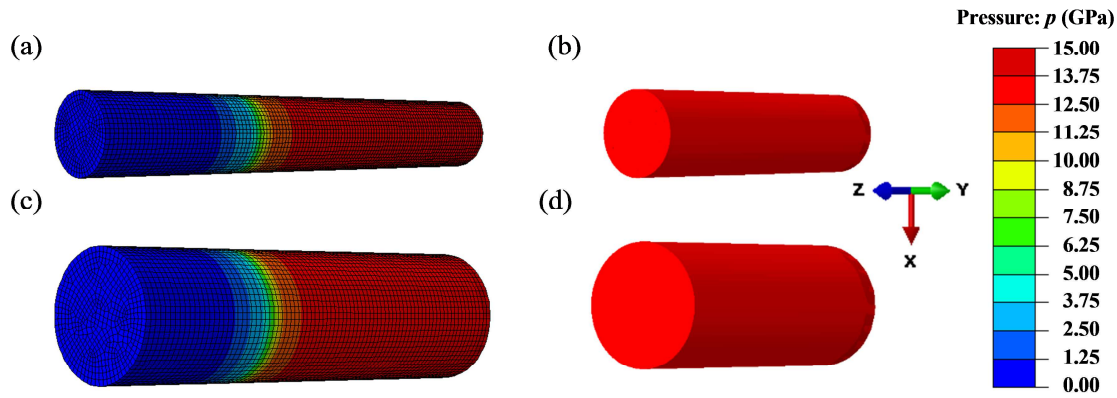


Fig. 5. Pressure distribution for the [0001] crystal at $t = 0.181 \mu\text{s}$ and the impact surface on the right end. (a) the 10 μm sample with 63384 elements; (b) cross section of the 10 μm sample at one-half length; (c) the 20 μm sample with 66801 elements; (d) cross-section of the 20 μm sample at one-half length.

Fig. 6 presents the distribution of parent material volume fraction for the half of sample. The maximum volume fraction of the parent material is localized at the region close to the impact plane due to edge effects and the nature of the interaction with the copper flyer plate which retards the formation and growth of deformation twins. From the impact plane to the free surface, the volume fraction of parent material decreases and inside of sample as shown in the middle plane, the heterogeneity of parent material volume fraction is small, where we can see slightly greater heterogeneity at the outer radius of the small sample than that in the larger

sample. In this paper, small sample means that the sample has a radius of $10\text{ }\mu\text{m}$ and the large sample with radius of $20\text{ }\mu\text{m}$.

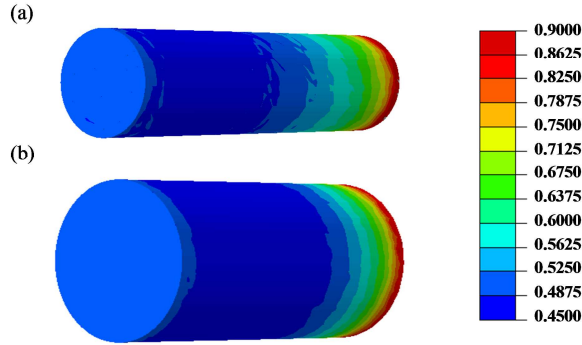


Fig. 6. Parent material volume fraction for the [0001] crystal at $t = 0.181\text{ }\mu\text{s}$ displayed in the half-section of the sample at the impact plane end. (a) $10\text{ }\mu\text{m}$ radius model; (b) $20\text{ }\mu\text{m}$ radius model.

Fig. 7 shows the distribution of one of six primary twin variants (number 1 twin variant as seen in the Fig. 7c). The volume fraction magnitude for this single twin variant displayed in Fig. 7 varies rather substantially throughout the volume of the material for both sized models. Since there is not inherent length scale introduced in the theory and no seeding of initial heterogeneity was done, this can be attributed to alterations in local deformation perturbed by small numerical variability leading to the pathways taken. Fig. 8 shows the field of volume fraction of the omega phase variant transformed from the number 1 primary twin variant. Recall that we follow the pathway for primary twinning as a precursor to structural transition from α to ω phase, as discussed earlier. The field displayed in Fig. 7 is then that leading to the results given in Fig. 8. As in Fig. 7, spatial variability of the ω phase volume fraction is notable. Once again, the influence of constraints at the impact surface manifest themselves in the results shown in Fig. 8.

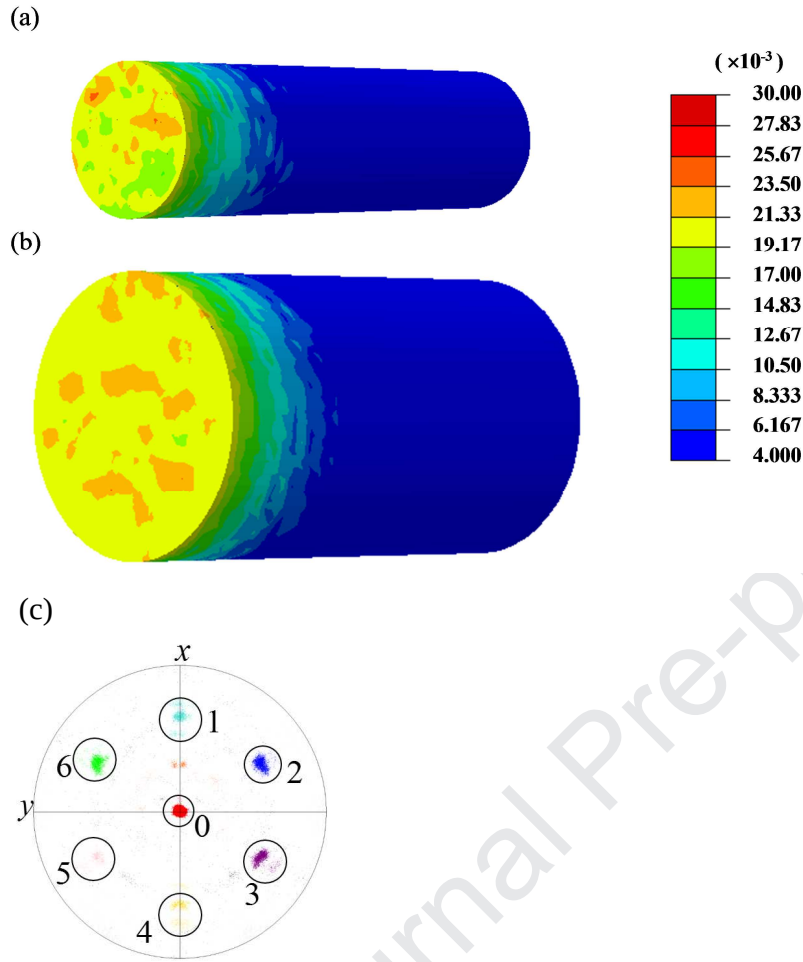


Fig. 7. Volume fraction of the number 1 primary twin for the [0001] crystal at $t = 0.181 \mu\text{s}$ for (a) the 10 μm model sample; (b) the 20 μm model sample; (c) [0001] pole figure from experiment and position numbers 0 and 1 corresponds to the locations of parent material and the number 1 primary twin respectively. Positions 2 – 6 are the remaining primary twin variants and their crystallographic position. The impact surface is at the right-hand end of the cylinders.

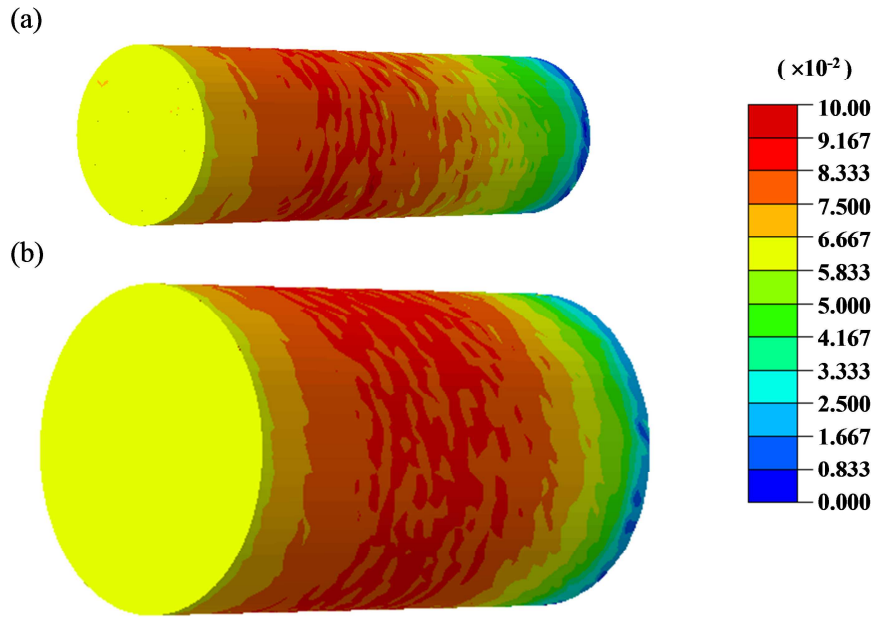


Fig. 8. the volume fraction of the omega phase variant transformed from number 1 primary twin for the [0001] crystal at $t = 0.181 \mu\text{s}$ for (a) the 10 μm radius model sample, and (b) the 20 μm model sample. The impact surface is at the right-hand end of the cylinders.

Figs. 9-10 presents the variations of pressure, von Mises stress, and volume fractions of material components at the centerline of the two cylindrical model samples in comparison with 1D results at the instant $t = 1.806 \mu\text{s}$. Note that the influence of impact surface constraints differs between the 1D and 3D models as illustrated in Fig. 9. Away from the impact surface however, there exists little difference in stress between the 1D and 3D models. The material state variable results are given in Fig. 10 as a function of distance from the impact surface. The volume fraction of parent α phase and ω phase among different sample sizes are very distinct in the region from impact plane to a distance of 0.5 mm away. For example, at $z = 0.25 \text{ mm}$ distance from the impact surface, the difference in the parent α phase volume fraction between the 10 μm and 20 μm samples is 10%. However, looking at primary twin variant 1 volume fraction results, there is not much difference between the three models even for the region close to the impact plane. This is because we set up a minimum volume fraction for twin variants of 0.005 preventing complete transformation of all primary twin material to ω phase (Feng et al., 2019) as shown in Fig. 10b.

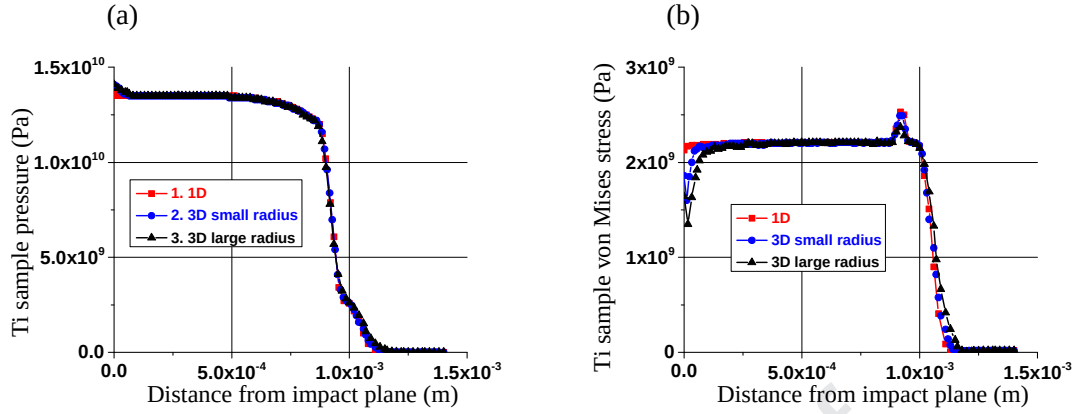


Fig. 9. Pressure and von Mises stress distributions for the [0001] oriented crystal at $t = 0.181 \mu\text{s}$ as a function of distance from the impact surface. Line 1 (red) is for the one-dimensional case. Line 2 (blue) is that taken along the cylinder centerline for the $10 \mu\text{m}$ model. Line 3 shows the values taken at the centerline of the cylindrical model for the $20 \mu\text{m}$ case.

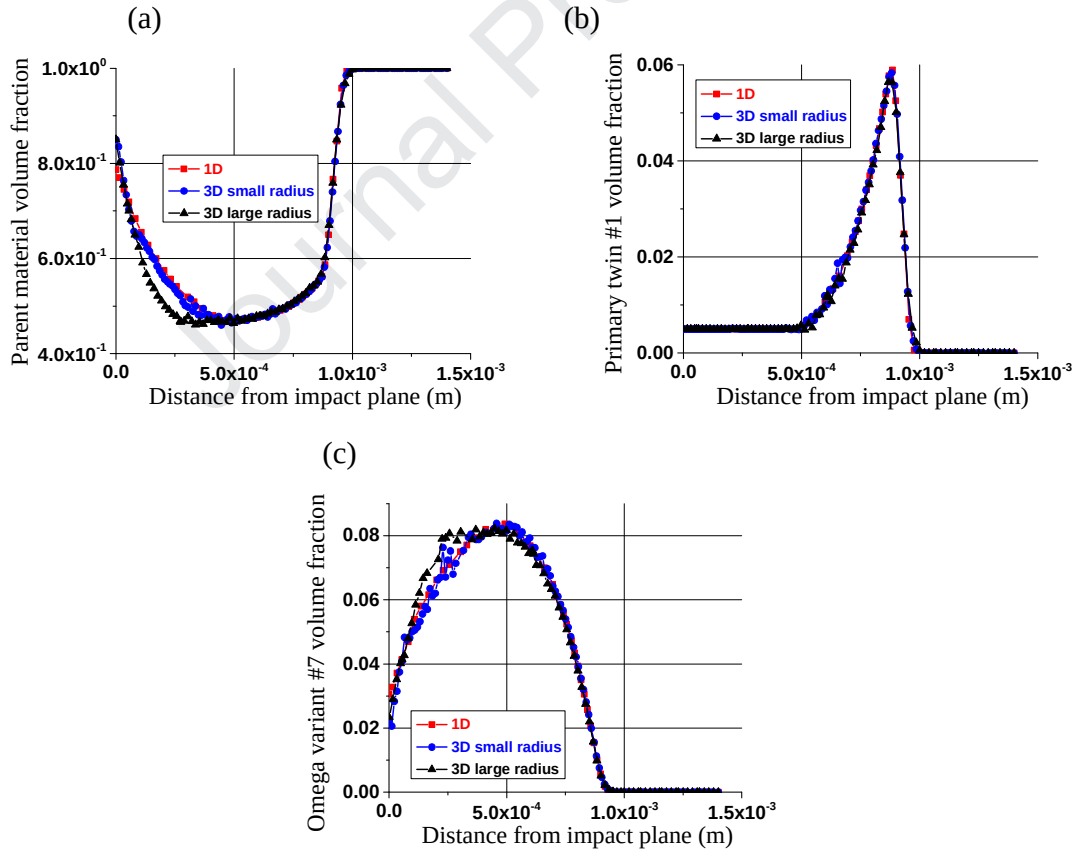
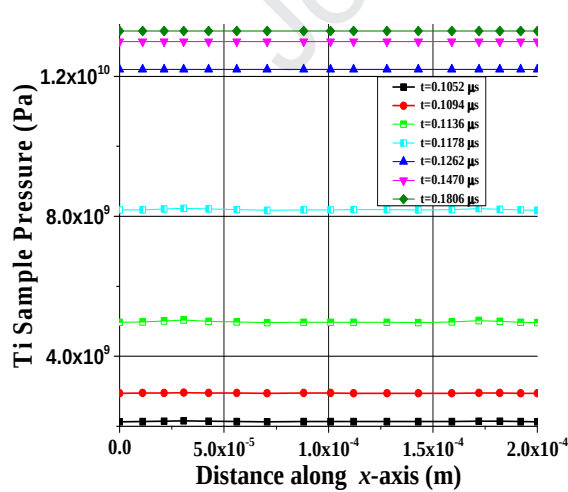


Fig. 10. Volume fractions of parent α material, the number 1 twin variant, and the ω phase variant #7 transformed from the number 1 primary twin for the [0001] crystal at $t = 0.181 \mu\text{s}$.

Line 1 (red) is for the one-dimensional case. Line 2 (blue) is that taken along the cylinder centerline for the 10 μm model. Line 3 are the values taken at the centerline of the cylindrical model for the 20 μm case.

Fig. 11 present the pressure and parent material volume fraction distributions for the [0001] crystal at different times through a diameter along the x axis at the middle plane between the free surface and impact plane for the large 3D model. For the pressure distributions shown in Fig. 11a, the variation through the diameter is small for the different times shown. The variation in the volume fraction of the parent α phase remains small for the early stages but grows with deformation as shown in Fig. 11b. Consistent with the contour plots examined earlier, the variability across the diameter at $t = 0.181\mu\text{s}$ begins to develop to a significant magnitude. The variability is a result of combined and coupled processes of slip, twinning, and phase transformation mechanisms.

(a)



(b)

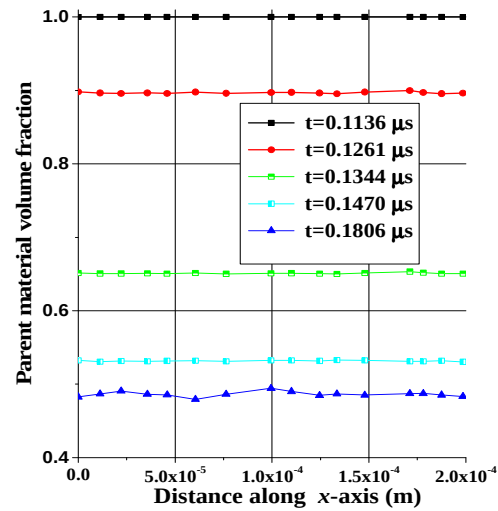


Fig. 11. (a) Pressure; and (b) parent material volume fraction distributions for the [0001] crystal at different time instants through the model diameter along the x axis at middle plane between the free surface and impact plane.

4.2.2 The $[10\bar{1}1]$ crystal

In this section, we will discuss the simulation results for single crystal Ti loaded in the $[10\bar{1}1]$ crystallographic direction. In the case of the [0001] crystallographic loading as discussed in the previous section, the c -axis was parallel with the cylindrical axis of the sample. Therefore, the rotational symmetry of slip and twinning systems would also tend to preserve the geometric symmetry of the cylinder during deformation. This is no longer the case for $[10\bar{1}1]$ crystallographic loading. Since the c -axis is now at an oblique angle with the axis of the cylinder, one should expect that the cylindrical geometry would not be preserved with deformation. This in turn causes heterogeneity of fields of stress and volume fraction of components in materials for the $[10\bar{1}1]$ crystal which is much severer than that in [0001] oriented crystal.

Fig. 12 presents the field of pressure for the impact plane half-end of the Ti sample cut between the free surface and impact plane. The variation of pressure in the half sample is around 7%, and is most visible at the impact surface. The asymmetric response of the single crystal of this orientation also manifests itself as the asymmetry in pressure loading response in comparison with that from the [0001] direction loading found in Fig. 5. This asymmetry is also reflected in the distribution in the volume fraction of the parent α phase given in Fig. 13. These results suggest that the variability in volume fraction reaches 45% between minimum and maximum values. The maximum volume fraction of parent α material is located around the impact plane due to boundary effects. The distribution in pressure and parent material between the small and large samples are different but the general nature of the heterogeneity is similar. In comparison, the degree of heterogeneity in the radial direction is much more severe in the case of the $[10\bar{1}1]$ direction loaded crystal than for the [0001] crystal as shown in Fig. 6. This suggests that a one-dimensional model may not be suitable for the $[10\bar{1}1]$ oriented crystal or any

crystallographic loading direction which does not preserve geometric axi-symmetry during loading. The radial direction (x -axis) variability for both pressure and volume fraction of the parent α phase is given in Fig. 14 as a line profile. These results do not capture the three-dimensional variability. The pressure variation given in Fig. 14a is quite substantial in comparison with the results in Fig. 11a. That fact that the slope of the lines becomes negative at different times is an indication of the 3D variability with time along the x -axis of measure. The volume fraction of the parent α phase material is plotted in Fig. 14b and once again significant variability is demonstrated. The difference is 4% at $t=0.252 \mu\text{s}$. The shape of the line profile volume fraction also changes with time which is another indicator of the 3D nature of the evolving fields and consistent with the results in Fig. 13.

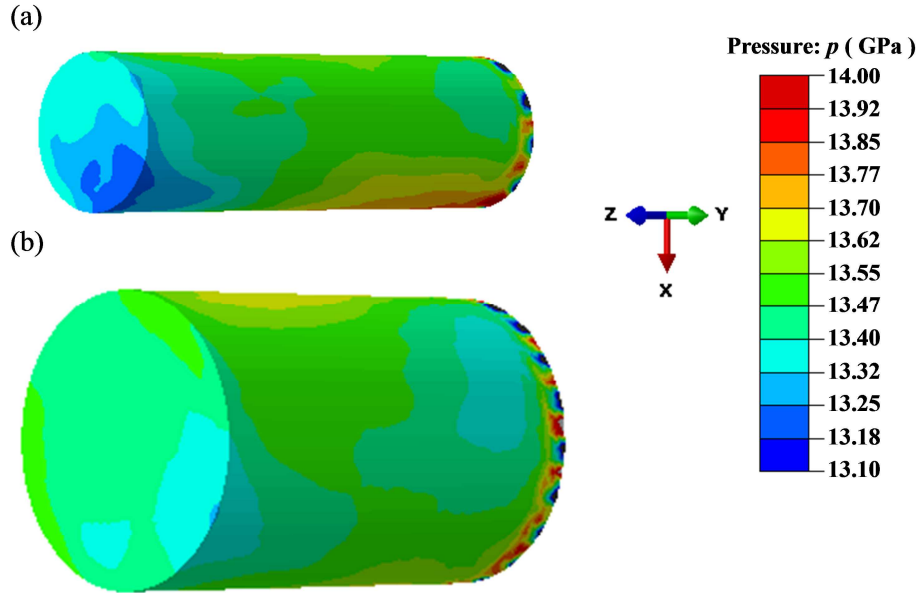


Fig. 12. Pressure for the $[10\bar{1}1]$ orientation crystal at $t = 0.181 \mu\text{s}$ for (a) the 10 μm radius sample model and; (b) the 20 μm sample model. The impact plane end of the models is shown sectioned at the center of each model.

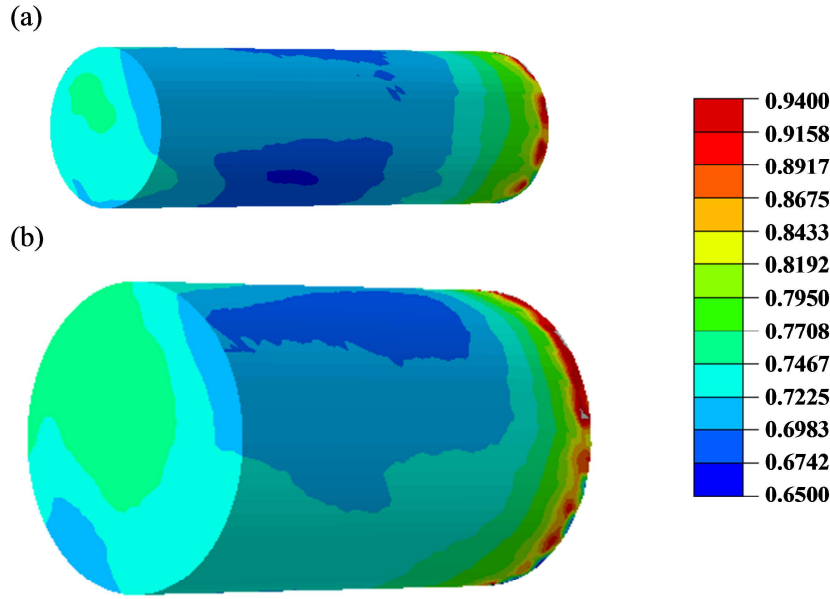


Fig. 13. Volume fraction of parent α phase material for the $[10\bar{1}1]$ orientation crystal at $t = 0.181 \mu\text{s}$ for (a) the 10 μm radius sample model and; (b) the 20 μm radius sample model. The impact plane end of the models is shown sectioned at the center of each model.

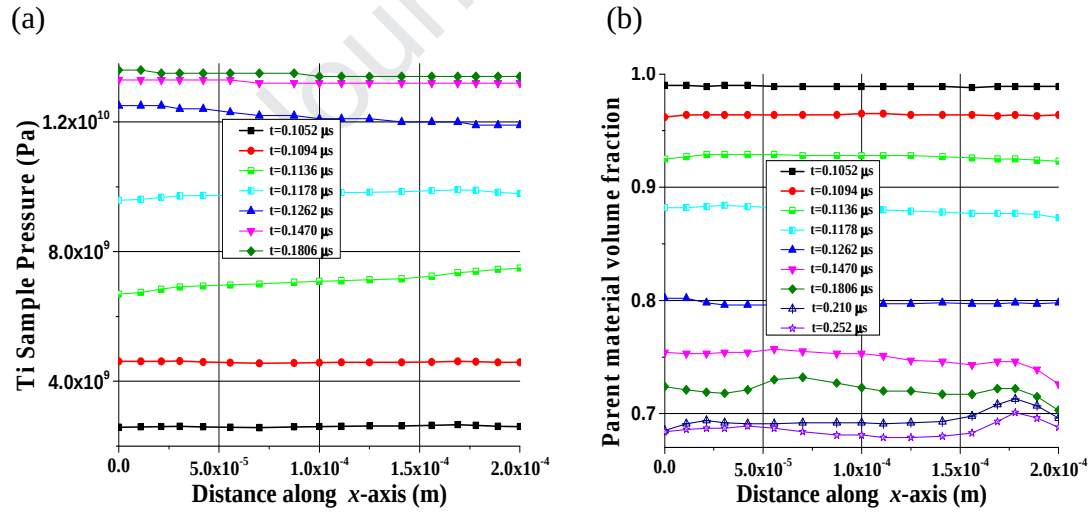


Fig. 14. (a) Pressure and; (b) parent α phase material volume fraction distributions for the $[10\bar{1}1]$ orientation crystal at different times along the x-axis at the middle plane between the free surface and impact plane.

Fig. 15 gives the pressure and von Mises stress plotted along the cylinder axis for the $[10\bar{1}1]$ orientation crystal. It is interesting to see in Fig. 15a that there is no obvious difference between 1D and 3D results. As the contour plots for pressure given in Fig. 12 illustrate, there is marked variation in pressure throughout the sample which is however not reflected along the centerline. The von Mises stress results along the given in Fig. 15b do indicate marked differences between the three simulation results. This von Mises stress difference is also reflected in the structural evolution variation illustrated in Fig. 13. The volume fractions of parent α phase material shows the difference between small sample and large sample to be around 7%, and so for this crystal orientation loading, the effects of problem size are not negligible. The results given in Fig. 16b showing the profiles of the primary twin variant number 1 volume fraction do not show significant differences, suggesting that secondary twinning is the principal reason for the differences observed in Fig. 16a between the three models. The other primary twin variant such as #2 in Fig. 16c also show little difference between 1D and 3D models.

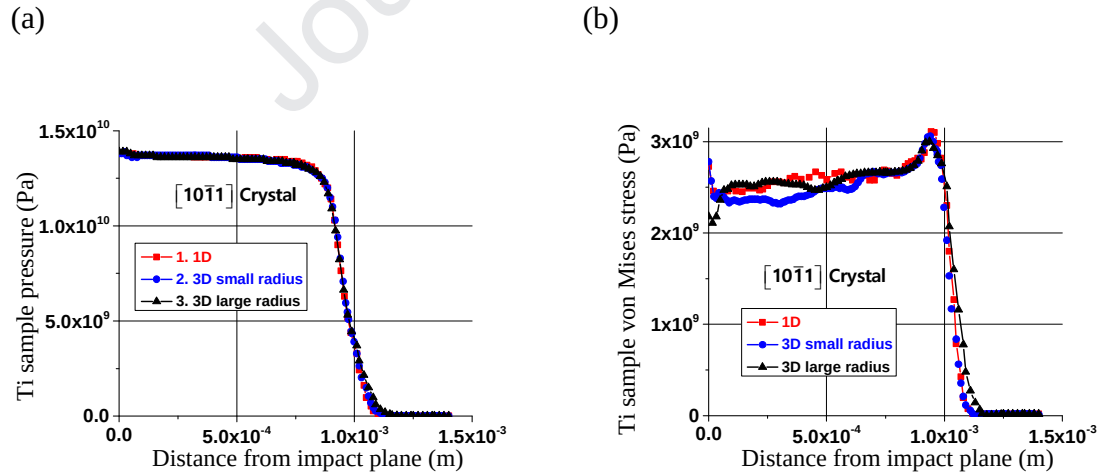


Fig. 15. (a) Pressure and; (b) von Mises stress distributions for the $[10\bar{1}1]$ orientation crystal along the center axis of the models. Line 1 (red) is for the one-dimensional case; line 2 (blue) is

from the 10 μm radius model; line 3 (black) is from the 20 μm radius model. Values in each of the two plots are taken along the centerline of the cylindrical sample for the 3D cases.

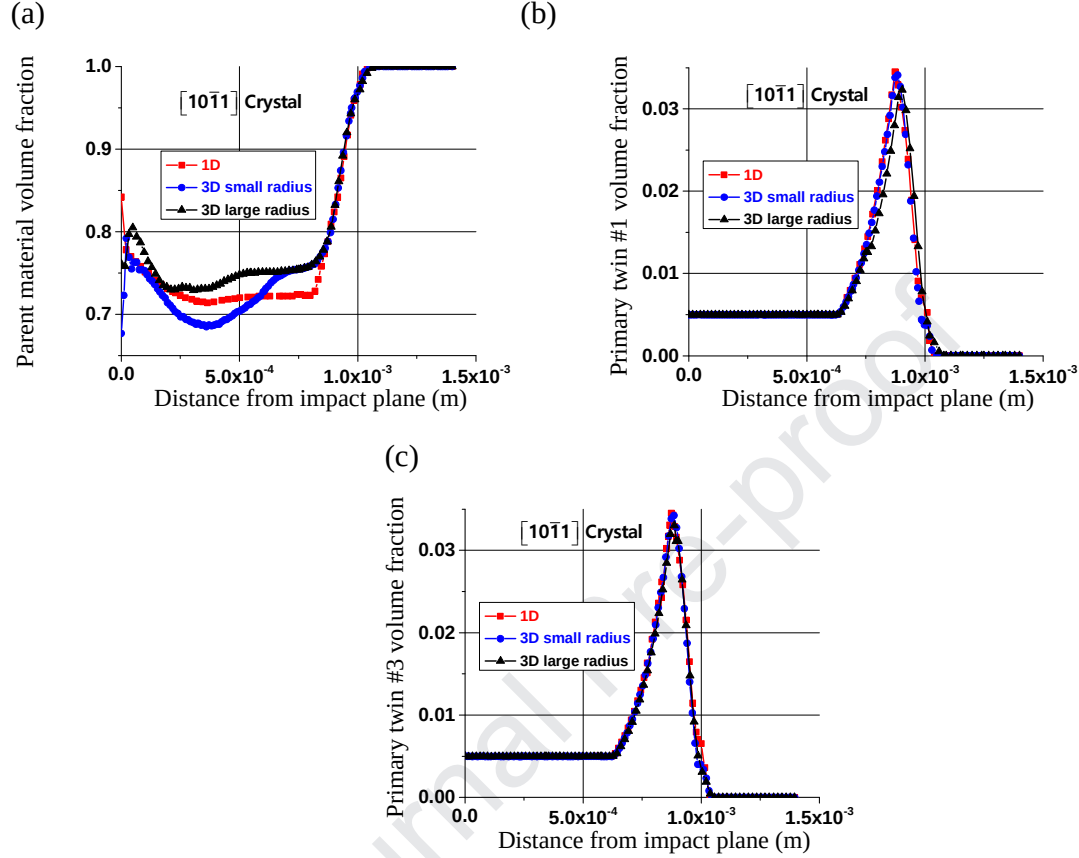


Fig. 16. Volume fraction of (a) parent α phase material and; (b) number 1 primary twin variant; (c) number 2 primary twin variant for the $[10\bar{1}1]$ orientation crystal at $t = 0.181\mu\text{s}$. Line 1 (red) is for the one-dimensional case; line 2 (blue) is from the 10 μm radius model; line 3 (black) is from the 20 μm radius model. Values in each of the two plots are taken along the centerline of the cylindrical sample for the 3D cases.

4.3 Three-dimensional bi-crystal model

In this section, we examine the results of simulations performed on a cylindrical bi-crystal composed of both $[0001]$ and $[10\bar{1}1]$ orientation crystals. This bi-crystal configuration forms an interface plane that is oriented along the axis of the cylindrical geometry using a computational model of radius 10 μm with 223,800 elements representing the sample. This bi-crystal interface is defined as an instantaneous change in crystallographic orientation between

elements across the plane of nodes that are shared between the elements on both sides. There are no degrees of freedom granted via the zero-thickness interface. Results showing pressure at $t = 0.181\mu\text{s}$ for both single crystal cases as well as that for the bi-crystal case is given in Fig. 17. We mention here that this bi-crystal interface does not represent a grain boundary as modification to the single crystal model to represent the dislocation mechanics in the vicinity of a grain boundary is beyond the scope of this work. As shown in Fig. 17, the distribution of pressure close to the shockwave front is different between the $[0001]$ and $[10\bar{1}1]$ orientation single crystal results. The pressure profile as viewed from the surface of each model differs along the axis of the cylinders which is expected due to differences in axial stiffness for the two crystal orientations. For the case of the bi-crystal, Fig. 17, the pressure from one crystal to the other, and pressure difference between the two crystals is relatively small, although slight differences exist. Comparisons in von Mises stress among the three models are given in Fig. 18. at $t = 0.181\mu\text{s}$. The results suggest that the von Mises stress is most uniform for the case of the $[0001]$ orientation and becomes less so in the case of the $[10\bar{1}1]$ orientation crystal. The bi-crystal results are quite interesting in that there is a clear and distinct difference in the two different crystals. The lingering stress condition behind the shock front is greater in magnitude within the $[0001]$ oriented single crystal. This is because the slip and twinning directions are completely different between the $[0001]$ and $[10\bar{1}1]$ crystals, therefore offering a source of significant incompatibility between the two grains.

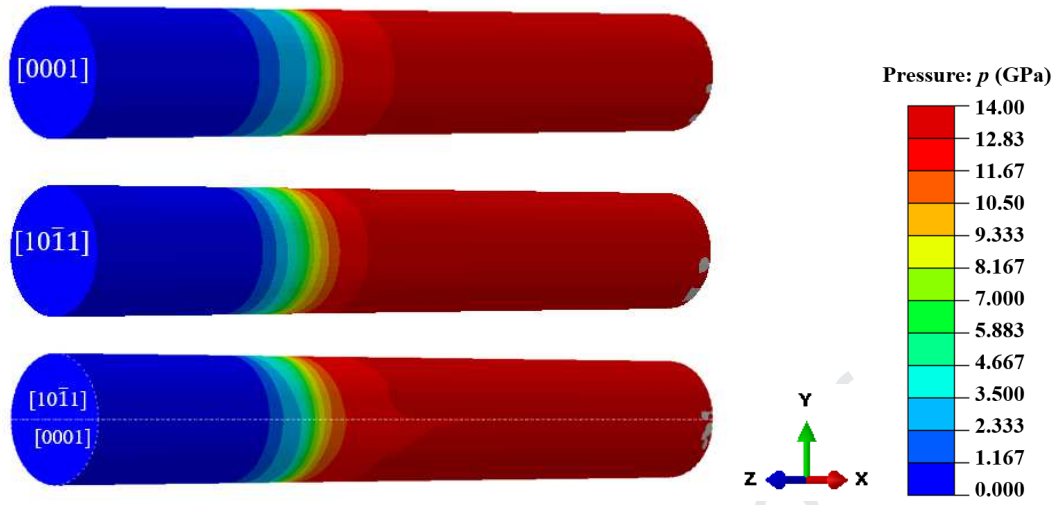


Fig. 17. Pressure distribution at $t = 0.181 \mu\text{s}$ for the $[0001]$ orientation crystal (top), the $[10\bar{1}1]$ orientation crystal (center), and bi-crystal (bottom). The cylinder radius is $10 \mu\text{m}$ for each of the three cases. Note that the entire length of the models is shown and illustrates the axial position of the shock wave at $t = 0.181 \mu\text{s}$ with the impact plane at the right end.

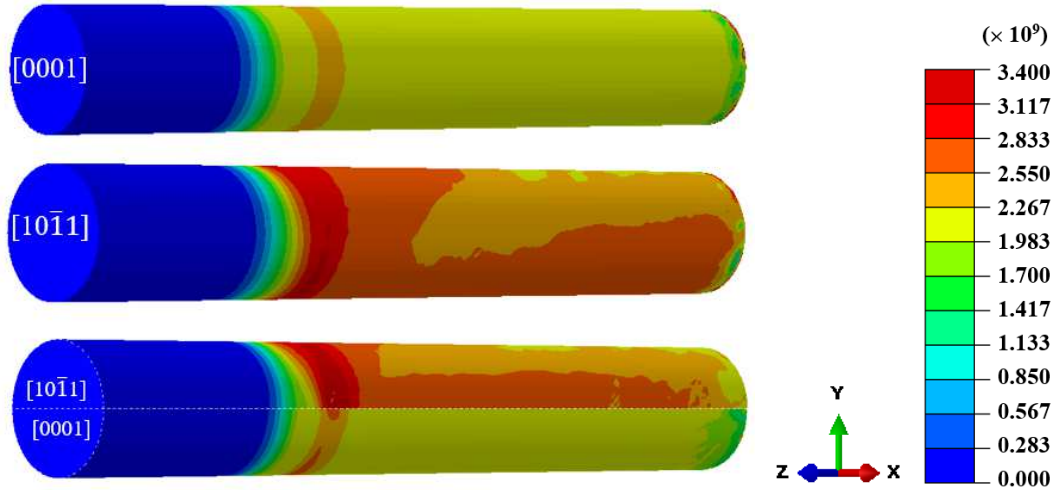


Fig. 18. von Mises stress distribution at $t = 0.181 \mu\text{s}$ for the $[0001]$ orientation crystal (top), the $[10\bar{1}1]$ orientation crystal (center), and bi-crystal (bottom). The cylinder radius is $10 \mu\text{m}$ for each of the three cases. Note that the entire length of the models is shown and illustrating the axial position of the shock wave at $t = 0.181 \mu\text{s}$ with the impact plane at the right end.

Fig. 19 shows the volume fraction of parent α phase material at $t = 0.181\mu\text{s}$ for the bi-crystal simulation. The difference in response of the two crystals is evident with substantially higher fraction of material retained as parent material beyond the shock wave front for the case of the $[10\bar{1}1]$ orientated grain contributing to combined incompatible behavior. Fig. 20 presents the profiles of volume fraction of parent α phase material along the axis of both $[0001]$ and $[10\bar{1}1]$ single crystals and bicrystal models as a function of distance from impact plane. Although the plots in Fig. 20 share a common profile shape with distance from impact plane, there are significant quantitative differences between the four curves.

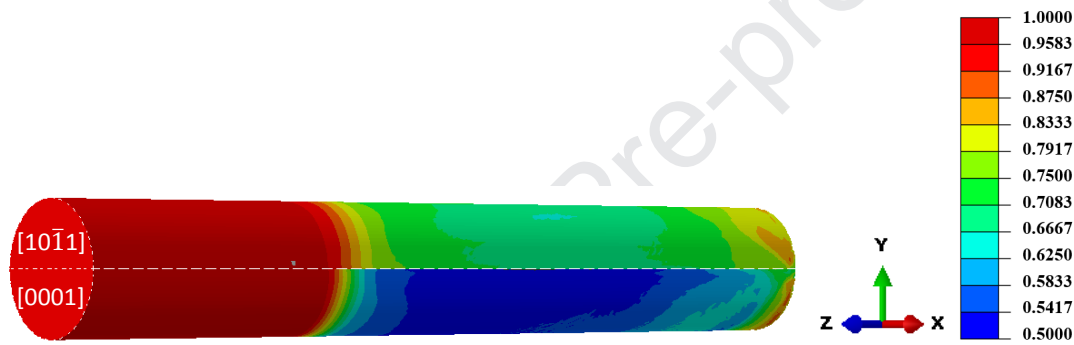


Fig. 19. Volume fraction of parent α phase material at $t = 0.181\mu\text{s}$ for the bi-crystal simulation. Note that the entire length of the models is shown and illustrates the axial position of the shock wave at $t = 0.181\mu\text{s}$ with the impact plane at the right end.

(a)

(b)

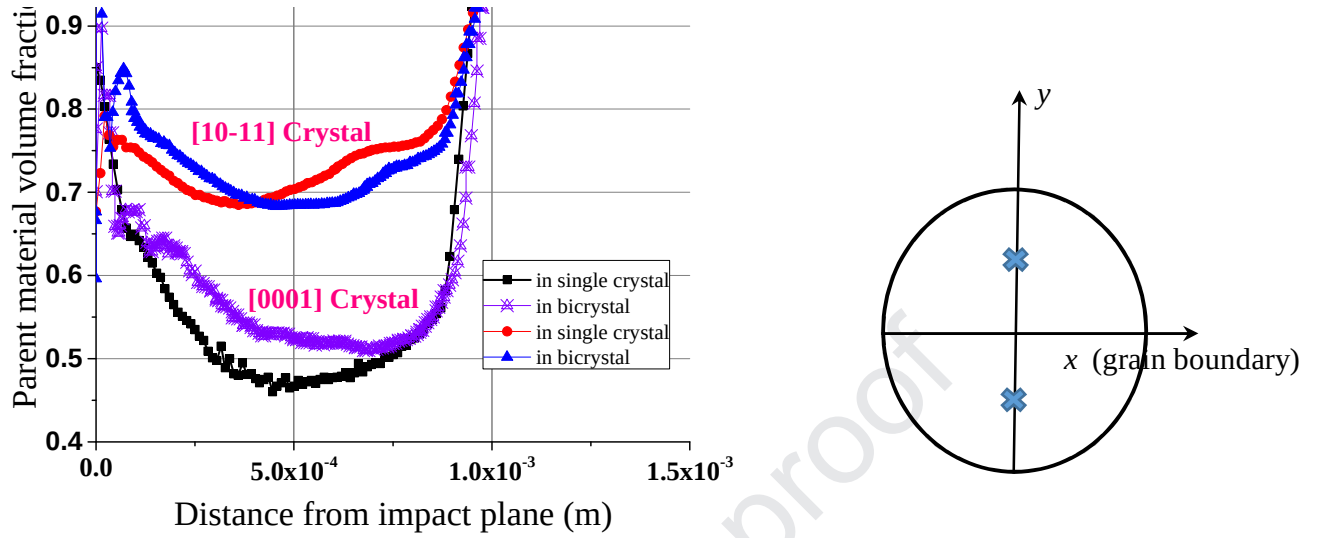


Fig. 20. Volume fraction of parent α phase material along the cylinder axis direction at $t = 0.181 \mu\text{s}$. For the bicrystal, the locations for curves in (a) are marked in (b). For single crystals, the location for curves in (a) are at the centerline of the cylinder.

The results for the bi-crystal simulations are shown in Figs. 21-23, in which the radius of the small sample is $10 \mu\text{m}$ (223,800 elements) and the large sample radius is $20 \mu\text{m}$ (224,000 elements) and the time instance is $t = 0.175 \mu\text{s}$. Fig. 21 presents the distribution of pressure in the bi-crystal, and the difference of pressure patterns between small and large samples is very small and size effect on stress is not very large, which is consistent with the single crystal case as shown in Fig 5 and Fig. 12. Close to the impact plane, the pressure shows some differences between small and large samples in Figs. 5, 12, and 21, which is caused by the sample interaction with the copper flyer that has different properties from the Ti sample. Fig. 22 shows the distribution of parent α phase material in the bi-crystal. Similar to the pressure distribution, close to the impact plane the difference in parent material between small and large sample is very different. However, for the [0001] orientation crystal in Fig. 22, the parent material distribution in the shockwave front is also very different for different sizes of samples. The size effect of parent material pattern is less obvious in the $[10\bar{1}1]$ orientation crystal, which is because the twinning of the $[10\bar{1}1]$ orientation crystal is less active and most of the material refrains from

undergoing twinning, in comparison with the case of the $[0001]$ orientation crystal. Fig. 23 shows the distribution of #2 primary twin in the bi-crystal. Similar to Fig. 22, the primary twin distribution is more affected by the sample size in the $[0001]$ orientation crystal than in the $[10\bar{1}1]$ orientation crystal, which is consistent with the case in single crystal case. The orientation of the $[0001]$ orientation crystal is more favorable to twinning than the $[10\bar{1}1]$ orientation crystal.

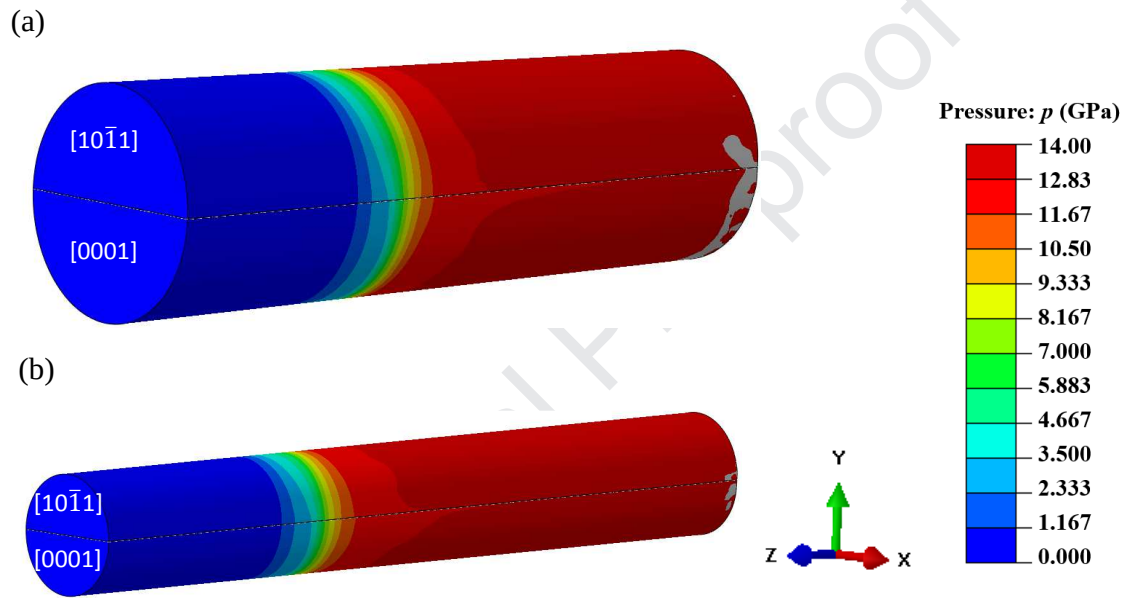


Fig. 21. Pressure distribution at $t = 0.175 \mu s$ for bi-crystal and the impact surface on the right end. (a) the 20 μm radius sample and (b) the 10 μm radius sample. The gray area close to impact plane is the region with pressure above 14 GPa.

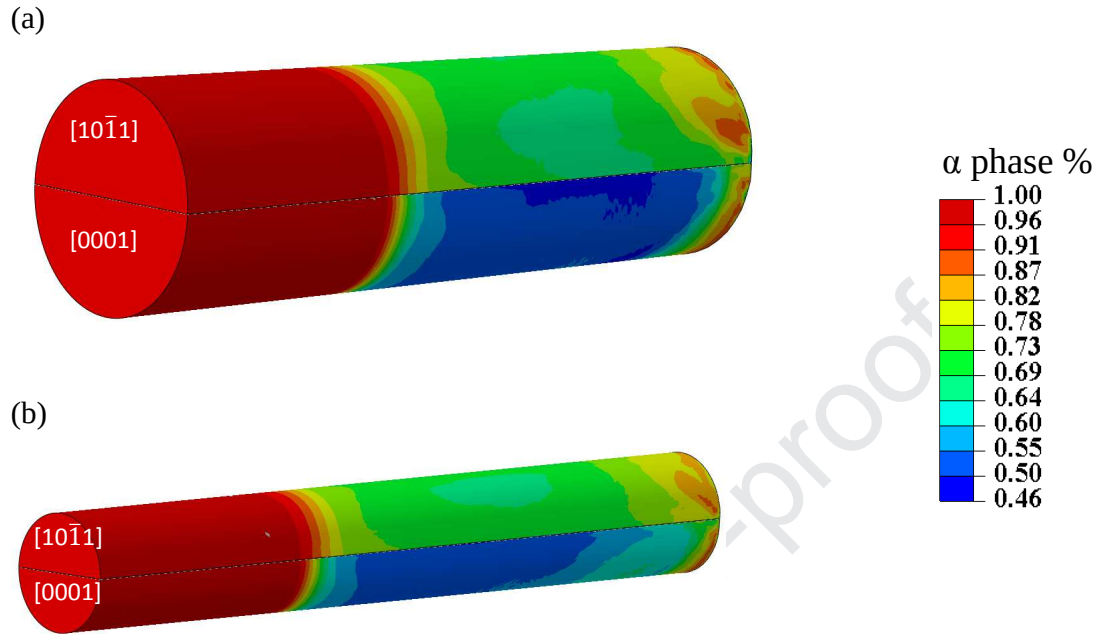


Fig. 22. Volume fraction of parent α phase material at $t = 0.175 \mu\text{s}$ for the bi-crystal. (a) the 20 μm radius sample and (b) the 10 μm radius sample.

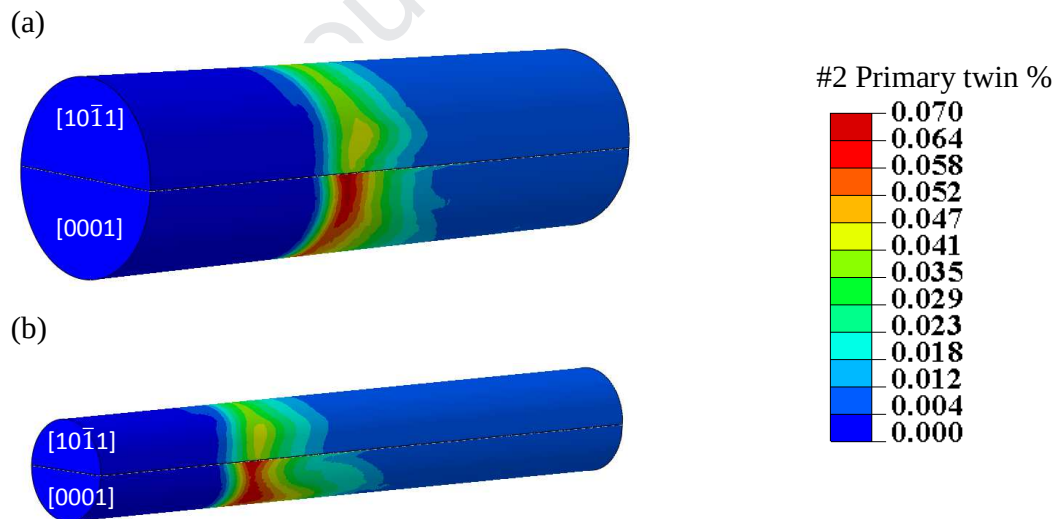


Fig. 23. Volume fraction of #2 primary twin at $t = 0.175 \mu\text{s}$ for bi-crystal. (a) the 20 μm radius sample and (b) the 10 μm radius sample.

5. Discussion

The work here has demonstrated the important relationship between dimensionality constraints imposed by the boundary value problem considered, the thickness of both the flyer plate and sample. Within the complex set of physics that the theory represents, many degrees of freedom in the equations are impacted by the three different boundary condition models which are presented and discussed in this work. These three cases change the size scale relationship between the sample dimensions and the transverse dimensions of the simulations. As the volume of the simulation is increased, in terms of the thickness dimensions, there exists a greater distance between the cylinder walls and center and therefore less constraint. This is also apparent in how the impact surface response is clearly different from that within the bulk of the volume given a similar number of elements and therefore Gauss points within the two differently sized models. The introduction of an interface between the two crystals also once again changes the relative length scales within the problem and the constraints to the system as well. This in turn is reflected in a different calculated response. The bi-crystal models again have similar numbers of element but more so than the single crystal models. As theories that we have presented here, and others in the community, continue to be developed and applied to larger numbers of grains and more comprehensive physical representation, the effect of these boundaries will then have an impact.

The heterogeneities developed on the simulations, particularly in the cases of the $[10\bar{1}1]$ orientation and bi-crystal results, are of considerable interest. Although perhaps perturbed by numerically generated variability, they are developed within a system of equations where local deformation pathways are spatially variable and impacted by boundary conditions. This is qualitatively similar to recent high-resolution dislocation mechanics simulations where patterns in local solutions were resolved (Arora and Acharya, 2019). The results point to solutions which take place and are affected by differing boundary conditions. As explicit twin representation becomes more tractable, we will also become more quantitatively accurate in representing local and spatially varying structure evolution for complex and coupled physics.

In the introduction, we offered a simple overview of the structural evolution which is observed to take place in high-purity Zr and Ti under dynamic loading conditions. The metallography images published of samples which were examined post-deformation (Cerreto *et*

al., 2013, 2014; Morrow *et al.*, 2016, 2017a,b) allows quantification of the characteristic length scales for the processes of dislocation slip, deformation twinning, and phase transformation. For the polycrystalline materials, the mean grain size certainly varies to some extent but for the Zr sample reported upon in Cerreta *et al.* (2013, 2014) the mean grain size appears to be on the order of 20 μm . The regions of deformation twinning generally span the diameter of the grain in the propagation direction but is only a fraction of the grain size transverse to the twin plane. The work of Morrow *et al.* (2016) and Feng *et al.* (2017) demonstrate that for the single crystal experiments, both primary and secondary twinning occurred. With secondary twinning, additional regions of orientations and interfaces are created with dimensions well below the original grain size of the material. Twinning as structural phase transformation is a nucleation and growth process and so there is a diverse length scale associated with those structural regions. The EBSD images reported in Cerreta *et al.* (2013) indicate that regions of ω phase begin as small and highly dispersed and for the sample with the highest level of retained ω , the remaining regions of α phase exist as long and thin laths with lengths on the order of the original grain size. Although the results reported in Cerreta *et al.* (2013) for the different sample conditions are not a simple progression of loading conditions, and thereby the deformation pathway is likely different for each sample, it does give a good idea of the change of structural heterogeneity occurring in this class of material (Zr, Ti) during shock loading. Our single view of dislocation structure of these materials is taken from Morrow *et al.*, (2016) where the TEM micrograph images suggest perhaps a reasonable degree of spatially uniform distribution with no formed dislocation sub-cells or dislocation density values reported. Given the varying characteristic length scales of each of the three inelastic processes observed in these materials, one can also perhaps expect the heterogeneity in stress to mirror that in the structure when loaded.

Although there are implied length scales within the theory via the different rate-dependent mechanisms, there are none that are explicit, except the average mobile dislocation loop radius $\bar{r}_{M\eta i}$, mobile dislocation velocity, $v_{\beta i}$, relative dislocation velocity $v_{A\eta i - B\beta j}$, and of course Burger's vector magnitude $b_{\beta i}$. The theory employed for dislocation slip is designed for applications of broad ranges of deformation-rate loading and takes a very physical approach to the representation of dislocation motion and interactions in comparison to convention. Although only a brief overview to the theory is presented here, more detail can be found in Hansen *et al.*

(2013) for fcc materials and Feng *et al.*, (2018,2019) for hcp materials. For the present case, given the Burger's vector difference with slip system type, this is reflected in our work on HCP Ti. Such an approach is appropriate here since more physical inference in comparison to the experimental results can be made and doing so also gives direct experience with an advanced physics model against experiments. Although including dislocation source creation was proposed by Hansen *et al.* (2013) and shown to be significant at very high loading rates, it has not been included here due to the relatively small amount of experimental data available and we assume sufficient number of mobile dislocations initially for the experimental conditions. The reasonable number of quantities within the model are physical and therefore contains a relatively low level of phenomenology. Employing such a model also provides a greater number of physical degrees of freedom in slip pathways when combined with the other deformation and transformation processes. This can in turn facilitate more spatial variability in computed material state such as seen in the results presented here.

HCP materials such as Ti ,Zr , Mg, and Be are well known to deform by pathways which include the mechanism of deformation twinning in addition to slip (e.g. Beyerlein *et al.*, 2010, 2011; Kumar *et al.*, 2016; Salem *et al.*, 2003; Gray, 1997; Capolungo *et al.*, 2009; Livescu *et al.*, 2019; Brown *et al.*, 2013). The results which have been presented here and related publications (Morrow *et al.*, 2016, 2017a,b; Feng *et al.*, 2018, 2019) considering high-purity titanium specifically suggest that deformation twinning plays a prominent role for these dynamic loading conditions. As the earlier discussed experimental results suggest, a majority of the material mass has likely undergone twinning. This process is believed to follow a nucleation, propagation, and growth system of discrete events that are driven by the structural heterogeneity and dislocation state in the system (e.g. Beyerlein *et al.* 2010, 2011; Niezgoda *et al.*, 2014; Jin *et al.*, 2019; Kumar and Beyerlein, 2020) although there is still much about that process which we do not yet understand. Since the interest in this work is to develop quantitative linkages with the available experimental results, it precludes use of discrete representation of deformation twins (e.g. Jin *et al.*, 2019; Kumar and Beyerlein, 2020; Ardeljan *et al.*, 2015; Cheng and Ghosh, 2015, 2017; Cheng *et al.*, 2018; Ghosh and Cheng, 2018; Chester *et al.*, 2016) at the present time. Our computational tools are not mature enough for large-scale problems and cases where there are both primary and secondary twinning taking place as our work suggests. This is a very important area of computational development as the deformation pathway leading to phase transformation

is also of significant importance. The representation of deformation twinning via a homogenized pseudo-slip model is a significant compromise. Even so, the physical pathways for deformation are represented on the same level as that for dislocation slip, albeit at a more phenomenological level due to a lack of understanding and computational capability.

Similar in concept to deformation twinning, structural driven phase transformation is believed to follow a nucleation, growth, and coalescence sequence in its progression. For the two group IV transition metals Ti and Zr in particular, the EBSD images given in Cerreta *et al.* (2013) give some insight to the characteristic length scales for at least for those loading conditions examined in Zr. Close examination of Fig. 1c in that publication shows very small and disperse regions of ω phase interspersed within parent α phase. Although there are resolution limitation for the scanning pattern used, the ω phase regions may likely be smaller in size than $1\ \mu\text{m}$ with an average spacing between ω phase regions of less than $5\ \mu\text{m}$. It would be of interest to better understand where within the parent α phase the ω phase regions may lie. That information is currently not available. Jones *et al.* (2017) performed a plate impact experiment on a polycrystalline high-purity Ti sample where the recovered sample retained 65% of ω phase. An EBSD image was reported showing a phase map over a square of approximately $150\ \mu\text{m}$ side length. The morphological relationship indicated isolated lath regions of α phase interspersed with the dominant ω phase with lath thickness on the order of less than $5\ \mu\text{m}$. Some interesting crystallographic texture data is also reported but we have not exercised it in our analysis here since we are focused on single crystal response. Large polycrystal simulations are planned for the future. In the formulation of the theory outlined in this manuscript, we hypothesized that the ω phase regions were formed only in prior twinned regions in keeping with the pathway observations made by Zong *et al.* (2014a) as a way to explain the observed large crystallographic rotation (85°) between the α and ω phases. In light of results presented here and those in Feng *et al.* (2019) indicate a systematic discrepancy between simulated and experimental pole figures for the $[0001]$ loaded crystal (Fig. 5 in Feng *et al.*, 2019). Although the orientation relationship between the parent α phase and the ω phase is not coincident, it is also not an 85° rotation as the MD simulations of Zong *et al.* (2014b) were indicating and as the theory predicts based upon this hypothesis. Given that the magnitude of plastic deformation for plate impact loading is not large, it is unlikely that plastic deformation after phase transformation could explain this significant

orientation relationship disparity and more work is necessary to explain. In particular, we know little about the plastic deformation behavior of the ω phase and especially with respect to the overall deformation pathway history.

This work has also not dealt directly with the topic of initiation events. Although less of a question for dislocation mediated plasticity for the loading conditions considered here, certainly twinning and phase transformation are believed to be strongly susceptible to nucleation conditions (Cheng and Ghosh, 2015; Jin *et al.*, 2019; Niezgoda *et al.*, 2014; Tomellini and Politi, 2019). These nucleation phenomena are also expected to be strongly dependent upon local heterogeneities existing within polycrystalline metallic materials and considered as extreme statistical events (Chen and Majda, 2018; Chen *et al.*, 2018). Grain boundaries and other types of interfaces within the material are expected to play a role in nucleation of events for polycrystalline materials.

6. Conclusion

This work follows in a line of work (Gray III, 1997; Greeff *et al.*, 2001; Morrow *et al.*, 2016, 2017a,b; Cerreta *et al.*, 2006a,b, 2013; Feng *et al.*, 2018, 2019; Livescu *et al.*, 2019; Zong *et al.*, 2014a,b,c, 2016) to understand the coupled phase transformation response of Type IV transition metal Ti under dynamic loading conditions in the presence of finite elasticity, dislocation slip, and deformation twinning. The results presented here show tangible impact of boundary conditions on the deformation pathway for the plate impact loading when the length of flyer and sample are accounted for and the impact interface is represented. The results are presented against available experimental data for single crystal samples of two different orientations with respect to the shock direction. These two orientations are $[0001]$ and $[10\bar{1}1]$. The experiments and simulations demonstrate clear differences in response of these two samples as the deformation pathway for the two oriented samples is significantly different given the highly anisotropic nature of the HCP material. These complex pathways are suggested to be responsible for the computed heterogeneity for the $[10\bar{1}1]$ orientated sample in particular given the asymmetry in loading at that orientation with respect to the axis of symmetry of the crystal structure. The presence of an intragranular interface is also shown to impact the response of each crystal for bi-crystal simulations using both orientations. These results suggest the importance in

more accurately representing the relative length scales for problems such as these when polycrystalline materials are being considered.

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Highlights

- Structural phase transformation in single crystal Ti is examined via numerical simulation employing a finite deformation thermodynamically consistent theory representing finite elasticity, dislocation slip, deformation twinning, and phase transformation.
- Numerical simulations are compared against plate impact experiments of single crystal high-purity Ti using the classical one-dimensional representation but also two three-dimensional models of differing size.
- Results show the importance of representing complex deformation physics in three-dimensions as the influence of boundary conditions affects the physical response displayed computationally.