An improved atomistic simulation based mixed-mode cohesive zone law considering non-planar crack growth

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A novel and improved atomistic simulation based cohesive zone law characterizing interfacial debonding is developed which explicitly accounts for the non-planarity of the crack propagation. Group of atoms in the simulation constituting cohesive zones which are used to obtain local stress and crack opening displacement data are determined dynamically during the non-planar crack growth as they cannot be determined apriori. The methodology is used to study the debonding of $\Sigma 5$-[2 1 0][0 0 1] symmetric tilt grain boundary interface in a Cu bicrystal under several mixed mode loading conditions. Simulations show that such bicrystalline specimen exhibits three types of energy dissipative mechanisms – shear coupled GB migration (SCM) away from the crack-tips, change in spatial orientation of GB structural units rendering highly disordered grain boundary near the crack tips and brittle intergranular fracture. Which combination of these three deformation mechanism will be active influencing the degree of non-planarity of the crack propagation at various stages of loading depends on the loading mode-mixity. As the ratio of shear component of the loading parallel to the GB plane and normal to the tilt axis with respect to the normal loading increases (thereby increasing the mode-mixity), overall strain-to-failure also increases and SCM tends to become the dominant deformation mechanism. Through this framework, analytical functional forms and parameters describing cohesive laws for both normal and shear traction as a function of the mode-mixity of the loading and crack opening displacement are predicted.

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1. Introduction and background

Nanostructured and nanocrystalline materials possess excellent properties for wide range of advanced technology applications. Owing to advances in nanotechnology research revealing their potential, there is a tremendous interest in considering them for several industrial sectors e.g. marine and aerospace industries, biomedical applications, microelectronic and SiP products, nuclear industry, defense and military applications (cf. Bringa et al., 2005; Grimes et al., 2008; Moya et al., 2007; Podsialdo et al., 2007; Roy et al., 2005; Traykova et al., 2006; Wang et al., 2002; Zhan et al., 2005). An important and distinctive characteristic of these nano materials compared with conventional composites is that interfaces in them occupy significant portion of the bulk volume i.e. ratio of hetero-interface area in nanocomposites and grain boundary interface area in nanocrystalline metals or ceramic to their bulk volume is considerably higher compared to their conventional counterparts. Due to such higher interface area-to-volume ratio, they often display distinctly different properties across the spectrum in comparison to their conventional bulk form (cf. (Gu and He, 2011; Le-Quang et al., 2010; Le-Quang and He, 2007; Paliwal and Cherkaoui, 2012)). Therefore, mechanistic understanding of deformation and fracture along and in the vicinity of interfaces in such material systems is of paramount importance to appropriately design and to predict reliability of the product. Among various interface-mediated deformation and failure mechanisms, modeling of interfacial debonding in nanocomposites (and intergranular fracture in nanocrystalline materials) have received considerable attention in the past. As the size-scale of interest in these composite-systems is within tens of nano-meters, incorporation of atomic level physics in models of deformation and fracture have become very important to realistically simulate their overall mechanical response. Historically, interfacial fracture of wide range of materials have often been simulated through cohesive zone modeling (CZM) in conjunction with the finite element method (FEM). The CZM concept was proposed by Barenblatt (1959) and Dugdale (1960) who regarded fracture as a gradual process. While no stress transmission occurs between fully separated crack surfaces, cohesive or fracture process zone ahead of them continues to transmit force between a pair of virtual surfaces in accordance with a phenomenological model. The cohesive tractions between these virtual crack surfaces, due to interatomic forces, constitute
resistance to crack propagation. Such phenomenological model aims at presenting mechanical response of this cohesive zone and is governed by a traction-crack opening displacement constitutive law (TDCL).

Conventionally, parameters for TDCL characterizing CZM for various types of interfaces are empirically obtained using estimates of fracture toughness, strength, stress vs. crack opening displacement, etc.; such estimates are further obtained through experimental or numerical studies. For example, Wei and Anand (2004) used cohesive interface modeling to study the deformation and fracture response of nanocrystalline nickel. Within CZM framework, they built elastic–plastic–grain–boundary interface model which accounts for both reversible elastic as well as irreversible inelastic sliding-separation deformations at the grain boundaries prior to failure. Key parameters characterizing CZM were obtained from experimentally measured macroscopic tensile stress–strain curves from specimens of electrodeposited nickel with grain sizes ranging from 15 to 40 nm. Tan et al. (2005) presented an experimental approach to determine the cohesive law for particle/matrix interfaces in high explosive PBX 9501. Using digital image correlation technique, they obtained stress and displacement around a macroscopic crack tip in PBX 9501 specimen under far-field tensile loading which was used to construct cohesive law characterizing interfacial debonding. More recently, Freed and Banks-Sills (2007) implemented a bilinear cohesive interface model representing transformation toughening zones between austenitic and martensitic phases in FEM to simulate crack growth in shape memory alloys. Crack resistance R-curves were obtained, which in-turn were used to determine parameters governing traction–separation constitutive law. We note that in all of these aforementioned cases, among many others, parametric fitting of TDCL were obtained from average response of thousands of micro-structural constituents of the specimen such as grains, grain boundaries, inhomogeneities, inclusions and other defects and does not represent the local response of the region surrounding the crack tip. It is therefore inappropriate to consider such methodologies, as representation of the constitutive behavior of interfacial debonding, or of intergranular fracture at the nano-scale – the phenomenon most pertinent to nano-materials. To accurately describe such phenomenon through CZM, parameterization methodology must imbibe localized nanoscale deformation mechanisms using appropriately designed experimental results or using atomistic simulations.

Several attempts have been made in the past describing methodologies to extract CZM parameters through atomistic simulations of interfacial failure. These methodologies can be classified into two distinct categories. Studies belonging to the first category presented atomistic simulations which describe key deformation mechanisms leading to final debonding of several types of bi-matter material system with intact interface (e.g. Awasthi et al., 2009; Gall et al., 2000; Komanduri et al., 2001; Spearot et al., 2004). Gall et al. (2000) used modified Embedded Atom Method (MEAM) to simulate of the deformation and fracture characteristics of an incoherent interface between FCC aluminum and diamond cubic silicon. Simulations were conducted under tensile loading; bulk stress and displacement of atoms in vicinity of the interface were used to obtain traction–displacement response. Spearot et al. (2004) developed internal state variable (ISV) framework that uses cohesive interface separation constitutive laws motivated by MD simulations. Simulations were presented for bimaterial system consisting of a planar, tilt nanograin boundary interface subjected to tension and shear deformations. More recently, Awasthi et al. (2009) presented MD simulations using the Consistent Valence Force Field (CVFF, describing atomistic interactions) to study nanoscale characterization of the force-separation behavior between CNTs and the polymer matrix. Separation mechanisms were studied for both opening as well as sliding modes and for each mode, cohesive zone parameters such as peak traction and energy of separation were evaluated. All these aforementioned studies consider overall system size between 2 and 8 nm and model interfacial decohesion as an adhesive failure. As noted by Yamakov et al. (2006), in order to obtain appropriate parameterization of CZM representing interfacial fracture, atomistic model must simulate mechanistic processes of crack initiation and propagation rather than that of adhesion. Moreover, unlike these approaches data must be extracted from regions in the vicinity of the crack tip where most of inelastic deformation is occurring rather than from entire simulation domain. Considering these limitations, several researchers have used a different approach (which constitutes the second category) to developed models of interfacial debonding through atomistic simulations of bimaterial systems with pre-cracked interface (Dandekar and Shin, 2011a,b; Krull and Yuan, 2011; Yamakov et al., 2006; Zhou et al., 2008). Yamakov et al. (2006) developed a cohesive debonding model using MD simulations of intergranular fracture in FCC Al with a pre-existing crack along the grain boundary (GB) subjected to mode-I tensile loading. One of the propagating crack-tips along the GB interface displayed brittle and the other displayed ductile fracture mechanisms. They presented a robust method using estimates of crack opening displacement with normal stress to construct a traction–separation law for both mechanisms. Yamakov’s framework (Yamakov et al., 2006) set a precedent for using such type of atomistic simulations to derive cohesive laws of interfacial debonding for wide range of material systems. Zhou et al. (2008) extended the methodology to derive a traction–displacement law for the fracture between two BCC type brittle materials with a weak pre-cracked interface under various mixed-mode loading conditions. Krull and Yuan (2011) developed an exponential traction–displacement law using parameters derived from quasi-static atomistic simulations of crack tip blunting and void initiation under mode-I tension. Dandekar and Shin (2011a) conducted atomistic simulations on a pre-cracked oxide/metal (Al2O3/Al) system under pure tensile and shear loading; they studied the effects of temperature and porosity on interfacial failure while deriving the traction–separation cohesive law from the data.

We underscore that entire framework to extract data from simulations as presented above is a significant improvement over Category-1 simulation approach; it nonetheless relies on the knowledge of the crack propagation path apriori. In this framework, crack propagation is considered to be strictly planar and is directed along the undeformed interface configuration. This assumption appeared reasonable as most simulations were conducted under conditions where during both stages of initiation and propagation, the crack is subjected to mode-I loading alone which mostly facilitates planar crack growth. Although mixed-mode loading conditions were utilized, they were used on a specific type of BCC bicrystalline system characterized by a brittle and weak interface (Zhou et al., 2008). It is noted by Lloyd et al. (2011) that the usage of a specific weak interatomic potential across the interfacial plane of such system might have contributed significantly to enforcing planar crack propagation. In atomistic model of more realistic material system, however, particularly with interface undulations and facets at the atomic scale – be it a dual phase bimaterial system, a single phase system with a GB interface, or a single phase homogeneous system – phenomena like localized crack kinking and deflection of the order of few nm normal to the interface (which is characteristic predetermined cohesive zone size in such models), localized crack branching and bifurcations, interface distortion under predominant shear loading condition, etc. are very likely to occur. Phenomenon of crack deflection can be exemplified by spalling in nano-scaled regions which has been reported extensively by many researchers in
structures like thin mono/multi-layered films, metal ceramic layered structures, wear & thermal protective coating to name a few (examples of few studies are (Dongfeng and Koji, 1994; Evans and Hutchinson, 1984, 1989; He and Hutchinson, 1989; McNaney et al., 1994; Okazaki et al., 2005). Due to elastic properties and coefficient of thermal expansion mismatch between the two material forming the interface and due to pre-existing residual and generation of thermal/internal stresses during thermal loading, interface cracks in such systems generally experience mixed-mode loading even under macroscopic tension. In such cases, interfacial crack tends to kink out and propagate in one of bulk materials. As the crack propagates beneath the interface, it creates a spell that incorporates the film and a portion of the underlying substrate (see e.g. Dronyi et al. (1988) and Okazaki et al. (2005). Another example is – in polymer/metal interface, often found in electronic packaging, not only adhesive failure (i.e. failure due to crack growth along the interface) but cohesive failure due to crack kinking in the polymer phase and propagating near the interface are often believed to be the cause of interfacial debonding (Noijen et al., 2009). It is therefore apparent that realistic scaled-down atomistic model of these systems to characterize interfacial traction–separation law, could very well exhibit such mechanisms of interfacial debonding at the atomic-to-nano scale particularly under mixed mode loading conditions. Such crack propagation mechanisms which still classify the fracture process as interfacial debonding, would make it very difficult if not impossible to determine the crack propagation path a priori.

Furthermore, in cases of a bicrystalline FCC system with a crack along a planar symmetric tilt GB (STGB) interface (a case of which is presented in this work) under shear loading, mechanisms like stress induced GB migration perpendicular to the interface and GB sliding parallel to the interface render extensive structural changes to the interface, making it highly non-planar. In nanocrystalline materials such GB mediated strain accommodative processes, which are believed to present two sets of a more general stress-induced migration process, significantly control the overall mechanical response of the polycrystal (see e.g. Mompiou et al. (2009), Schiotz and Jacobsen (2003), and Yamakov et al. (2004). In most (100) and other types of STGBs in a bicrystals, shear coupled GB migration is a reminiscent of collective glide of GB dislocations (see e.g. a coupling model describing shear-coupled GB migration by Cahn et al. (2006a) and Cahn and Taylor (2004) and experimental observation of the phenomenon in various Al bicrystal with (1 10) STGB by Gor-kaya et al. (2009) under shear stress acting normal to both the GB plane and the tilt axis of STGBs. These nano-sized intergranular cracks severely hinders such GB migration by pinning the GB dislocations in the vicinity of the crack-tips. It consequently causes the GB to bow-out, rendering the interface curved and non-planar. This further renders non-planar crack propagation as the system is subject to continued mixed-mode loading (more details on the mechanism are presented later in the paper). On the other hand, with regards to GB sliding, it has been reported that depending on the GB structural units GB sliding of several (1 10) type STGBs subjected to predominant shear loading is caused by events including local atomic scale shuffling in the vicinity of the GB, stress assisted free volume migration within the GB and nucleation of partial or extended dislocations from the GB to the grain interior (refer to e.g. Sansoz and Molinari (2005) and Warner and Molinari (2008). This inevitably renders heavily deformed and non-planar GB interface, and most likely causing the crack to deflect from its originally anticipated path under continued loading.

Hence, it is quite apparent that under such situations pertaining to most realistic interfacial debonding of large class of material systems, aforementioned methodology in its present form is not appropriate to determine TDCL. Therefore, to improve the fidelity of atomistically derived CZM we present a novel methodology which explicitly tackles such issues caused by non-planar crack growth by dynamically determining the cohesive zone regions as the crack progresses upon continued mixed-mode loading. Unlike previous atomistic models, these cohesive zones are not determined just at the beginning of the simulation. We describe the methodology in the next section where we use it to study the interfacial fracture of a Cu bicrystal with a (001) type STGB subjected to several mixed-mode loading conditions. This is followed by a results and discussion section of this case, and finally by a summary of the work.

2. Atomistic simulation methodology

2.1. MD model and loading conditions

Simulations were conducted on a Cu bicrystal with a Σ5 (210)/[001] STGB interface at 1 K temperature. Simulation methodology discussed in this work can also be applied on systems at higher temperatures of interest and would be a subject of later study. We, however, note that very high temperatures with excessive thermal oscillations of atoms can cause high degree of interface distortion, atomic disorder and shuffling. Upon external loading, this may cause excessive stress concentration (even in the vicinity of uncracked interface) resulting in large cracks/voids nucleation of size comparable to the pre-existing interfacial crack accompanied by excessive blunting of the existing crack tip. In such cases, failure is more like an interfacial rupture where a single major propagating crack front does not exist. Under such circumstances, it may not be appropriate to model interfacial failure by using conventional CZM framework which is defined for steady state crack propagation accompanied by small scale plasticity/micro-voids/micro-cracks constituting the process-zone. However for intermediate temperatures, the methodology is still applicable. Few important changes example choosing the appropriate cohesive zone size and spatial and temporal averaging of the data (as discussed in subsequent sections) may need to be altered depending upon the system. For example, Dandekar et al. have used the methodology to extract CZM law characterizing interfacial debonding on Al/Al2O3 system (Dandekar and Shin, 2011a) and Al/SiC system (Dandekar and Shin, 2011b) at temperatures as high as 873 K.

The interaction among Cu atoms is characterized by the many body embedded atom method (EAM) interatomic potential from Mishin et al. (2001). Following the coincident site lattice (CSL) theory, optimized structure with a [001] STGB is created by placing Crystal-I on top of Crystal-II such that x- & y-axis are aligned along [1–20] and [210] crystallographic directions, respectively of the Crystal-II; z-axis is the tilt axis and is aligned with [001] crystallographic direction of both crystals. Crystal-I is oriented such that it is the mirror image of Crystal-II with respect to the x–z plane (which is the [210] crystallographic plane). This renders the horizontal x–z plane as the STGB plane, with [100] directions of both FCC crystal making an angle 53.13° in the counterclockwise direction. The energy minimization is conducted with LAMMPS simulation software (Plimpton, 1995) using conjugate gradient method. Periodic boundary conditions were used along the STGB plane i.e. along x- and z-axis and non-periodic boundary conditions, along y-axis. This results in two surfaces (top and bottom) and one GB interface in the middle of the specimen normal to y-axis. Several initial configurations are tested by shifting the upper grain with respect to the lower grain so as to obtain the lowest energy state of a GB configuration after atomic relaxation. After statics simulation for energy minimization, system was dynamically equilibrated by conducting MD simulations for 40 ps under isothermal-isobaric (NPT) ensemble. Time step used for this simulations and for others, described later in the work, was chosen as 1 fs. Isobaric conditions
of zero pressure were used along x- and z-axis and isothermal condition with temperature of 1 K was maintained using Nose–Hoover thermostat. Position and velocity of each atom were obtained by time integration of the corresponding non-Hamiltonian equation of motion (for more details on the ensemble and equation used, refer to LAMMPS documentation http://lammps.sandia.gov and also Plimpton (1995)). Fig. 1 presents the optimized structural units of $\Sigma 5$ (210)//[001] STGB between crystals 1 & II forming the bicrystalline system with origin placed at the center of the GB plane. Crystallographic orientations of both crystals are also given in the figure. Considering the computational cost, overall size of the system was chosen as follows – 500 Å (length) along x-axis, 360 Å (height) along y-axis and 7.23 Å (thickness) along the z-axis. Results for cases of predominantly shear and tensile loading (discussed subsequently) obtained by using thicker specimen were not significantly different from those obtained using these system dimensions. The reason simply is because under loading conditions considered in this work, there are no additional inelastic deformation mechanisms activated (other than those which are discussed later) in thicker specimens for this type of bicrystalline Cu with [001] STGB interface. Hence specimen dimensions chosen for this study are deemed appropriate. We note that $\Sigma 5$ (210)//[001] STGB is a high angle grain boundary composed of edge dislocation which are ‘closely-packed’ compared with low angle STGBs consisting of array of widely separated discrete dislocations (Cahn et al., 2006b). As has been established from previous studies e.g. Cahn et al. (2006b) and Molodov et al. (2007), Frank Bilby equation (FBE) provides two feasible solutions for {001} STGBs for their effective GB dislocation content. These two solutions (as functions of tilt angle $\theta$ which is the acute angle between [100] crystallographic directions of the two grains) correspond to Burger’s vector of GB dislocations. First solution corresponds to Burger’s vector along [010] direction (with [010] slip-plane to the left of GB normal direction), and the second solution, along $\pm\{110\}$ direction (with $\{110\}$ slip-plane to the right of GB normal direction) of the reference lattice. The reference lattice is aligned with Crystal-I for first mode and with Crystal-II for the second mode of dislocation glide. These solutions represent dual behavior characterizing two different mechanisms of dislocation glides in two different directions. Collective glide of these GB dislocation in either of the two modes under external shear loading results in the motion of entire STGB – a well known GB mediated strain accommodative mechanism termed as shear coupled GB migration (Cahn et al., 2006a).

At low temperatures, either of these two competing coupled slip modes – (100) Mode-I or (110) Mode-II, can be activated, depending upon the magnitude of the resolved shear stress on slip plane and along slip direction of the respective mode. This implies that following condition – $\tau_{PSR}\sigma_{c1}(\theta) \geq \sigma_{c2}(\theta)$ (where $\sigma_{c1}(\theta)$ is the applied stress, $\sigma_{c2}(\theta)$ is the respective threshold value of the resolved shear stress. $\tau_{PSR}$ is the applied shear stress, $\mu d(100)/2$ is the Schmidt factor for the slip plane and slip direction of Mode-i, and $\sigma_{c2}(\theta)$ is the respective threshold value of the resolved shear stress) – must be satisfied to activate a particular coupling mechanism (Cahn et al., 2006b). In this equation, $\tau_{PSR}$ is the applied shear stress, $\mu d(100)/2$ is the Schmidt factor for the slip plane and slip direction of Mode-I, and $\sigma_{c2}(\theta)$ is the respective threshold value of the resolved shear stress. $\sigma_{c1}(\theta)$ for high angle GBs is analogous to the critical resolved shear stress for low angle GBs which is proportional to the glide component of the Peach–Koehler force required to initiate the collective glide of the arrays of GB-dislocations. Schmidt factor for Mode-I GB migration is $\sin(\theta)$ (it equals 0.6 for $\Sigma 5$ (210)//[001] STGB) and for Mode-II is $\cos(\theta)$ (it equals 0.8 for $\Sigma 5$ (210)//[001] STGB). This condition was assumed to be applicable for both low and high angle (001) STGBs at low enough temperatures (Cahn et al., 2006a). It is also noted that upon application of positive far-field shear stress $\tau_{PSR}$, Mode-I results in the GB migration along $+y$-direction, whereas Mode-II results in GB migration along $-y$-direction, thereby producing pure shear in the traversed lattice region. Cahn et al. (2006a) demonstrated that $\Sigma 5$ (210)//[001] STGB exhibited (1 1 0) Mode-II migration mode for temperature up to 1000 K (refer to Figure 8 of Cahn et al. (2006a) for Cu < 0 0 1 > STGBs). They believe that this is due to higher Schmidt factor and lower critical resolved shear stress associated with Mode-II as compared with Mode-I GB migration for $\Sigma 5$ (210)//[001] boundary (for more details refer to Section 10 of Cahn et al. (2006a)). We however note that in atomistic simulations of similar specimens with very large lateral dimension (i.e. along tilt axis) it has been reported that GB migration does not happen uniformly over a large area as is seen in cases with ‘thinner’ specimen considered in this study (see e.g. Cahn et al. (2006a) and Warner and Molinari (2008)). In very thick specimens, the early stages of GB migration is usually accompanied by a nucleation of the initial GB disconnection loop, a critical sized interfacial line defect of a dislocation character with a migration step (termed as an ‘embryo nucleation’ by Cahn et al. (2006a)); this loop spreads across the GB and eventually annihilates itself through the boundaries in the horizontal plane. This, however, is not the case with thin specimens.

Fig. 1. Optimized $\Sigma 5$ (210)//[001] symmetric tilt grain boundary between crystals 1 & II forming the bicrystalline system with origin placed at the center of the GB plane.
where the boundary displacements occur uniformly over the entire GB area. Although, for block thickness up to 3 nm, no plastic deformation due to dislocation emission from the crack-tips or from intact GB has been reported even under pure shear loading of three types of bicrystalline Cu with $\Sigma (310)/[001]$, $\Sigma 17 (530)/[001]$ and $\Sigma 41 (540)/[001]$ STGB interface (Luque et al. 2009).

We note that in this case of bicrystal Cu with $\langle 001 \rangle$ STGB interface, none of the 12 FCC slip systems are operational. For example, in $\langle 011 \rangle$ STGB interface there are 2 operational slip system in each bicrystal (as is evident in the work of Yamakov et al. (2006)). $\langle 001 \rangle$ STGB interface was chosen in the present study because the primary energy dissipative mechanism is through shear coupled GB migration under far field shear loading without the presence of interfacial crack (mixed-mode loading with tensile stress component in addition to shear eventually cause interfacial decohesion after some GB migration). In the presence of intergranular crack this GB migration becomes the predominant source of non-planar crack propagation (Section 3 contains more details). Primary objective of this study is to develop a computational methodology to deal with non-planar crack growth while estimating the CZM parameters from atomistic simulation. $\langle 001 \rangle$ STGB interface was ideal to demonstrate the effectiveness of the present framework, and at the same time it was simple enough not to involve other inelastic deformation processes involving dislocation emission from the crack tips. We note that similar to other frameworks, this methodology is perfectly capable of handling decohesion of other types of GBs e.g. $\langle 011 \rangle$ type of STGB which allows up to 4 slip systems to be activated, and allows other types of inelastic energy dissipative mechanisms to be activated like GB sliding accompanied by partial dislocation nucleation, atom-shuffling, etc. (Yamakov et al. 2006).

After dynamic equilibration of the bi-crystal specimen, an atomically sharp inter-granular crack was introduced by removing an atomic layer from the GB plane from the left and right side of the specimen across 60 Å (see the schematic of the specimen in Fig. 2). Due to periodic boundary conditions along x-axis, this results in an array of infinite inter-granular crack of length 120 Å. Interaction among atoms in regions 1 & 2 (see Fig. 2) were also turned-off during entire course of the simulation; all other atoms are allowed to interact with each other. This approach to screen the interaction among atoms across the crack-region has been used before by Yamakov et al. (2006) and by Zhou et al. (2009) to introduce a planar crack in their model. We note that unlike Zhou et al. (2009) who compute the neighbor list only once – at the beginning of the simulation, we have used the default neighbor-list computation condition implemented in LAMMPS. Therefore the neighbor list is recalculated once some atoms move more than half the skin distance of the atom. After the introduction of the inter-granular crack the system is subjected to further energy minimization and subsequently to dynamic equilibration for 40 ps under similar NPT ensemble as described above. Next, this equilibrated structure is divided into three regions – two layers Top and Bottom, classified as fixed-atoms layers where boundary conditions are applied (see those colored in black in schematic of Fig. 2) and the third region, classified as dynamic-atoms region, is sandwiched between Top and Bottom layer. These layers do not participate in computing data from the simulation and serve only to subject the dynamic atoms-region to the desired mixed-mode loading. Desired loading conditions are imparted by means of constant boundary velocity as follows. The Bottom fixed-atom layer is held fixed i.e. velocity of every atom in the region is zero, and velocity of every atom in the Top fixed-atom layer is given as $V = (\ddot{e}_{10x} + \ddot{e}_{17y})L$. In this equation, $\ddot{e}_{10x}$ and $\ddot{e}_{17y}$ are shear and tensile strain-rates, respectively and $L$ is the initial height of the dynamic-atoms region. In the simulation $\ddot{e}_{00} = \sqrt{(\ddot{e}_{10x})^2 + (\ddot{e}_{17y})^2}$ was chosen to be $2 \times 10^8$ s$^{-1}$, typical order-of-magnitude of the strain rates in most MD simulations. Loading angle $\theta = \tan^{-1}(\ddot{e}_{10x}/\ddot{e}_{17y})$ is varied from $0^\circ$ to $85^\circ$ to impart

![Fig. 2. Schematic presenting a case of planar crack propagation (on the left) and another case on non-planar crack propagation (on the right). Planar crack growth is assumed in several studies of interfacial debonding and allows the determination of group of atoms constituting cohesive zones apriori. For the case of non-planar crack growth, as shown on the right, cohesive zones are determined dynamically as the crack propagates because they cannot be determined at the beginning of the simulation.](image-url)
mixed-mode loading from pure tensile ($\theta = 0^\circ$) to predominantly shear ($\theta = 85^\circ$). Simulations were conducted for seven values of $\theta$ as listed in Table 1 which also includes shear and tensile velocities and strain-rates, respectively for each simulation. The position and velocity of atoms constituting dynamic region is computed by solving Newton’s equation of motion under the condition that box dimension along x- and z-direction remain fixed. Temperature of 1 K is controlled by using Nose–Hoover thermostat.

2.2. Determining cohesive zones dynamically

To construct an analytical cohesive zone model of GB decohesion as a function of mode mixity, traction–displacement data characterizing resistive cohesive forces vs. the separation of surfaces is required. First step to obtain such data from atomistic simulations is to locate the crack tip (at every desired simulation time-step) to determine the appropriate ‘collection of atoms’ ahead of this tip from which the data is extracted. Such group of atoms constitute a cohesive zone at continuum level where inelastic deformation is believed to occur causing damage and complete decohesion. As we know that decohesion is not instantaneous but is a result of a process – from elastic deformation to a damaged or incomplete/transient decohesion state, and finally all the way to complete separation. In this work we define the location of the crack tip at continuum level as the location where the average potential energy of group of atoms constituting continuum crack-tip region is greater than a threshold value ($u_0$). Atoms constituting fully cracked surface have higher average potential energy ($u_0$) than those constituting bulk ($u_0$) or those constituting bonded interface ($u_1$); $u_0$ is chosen such that it is closer to $u_0$ than to $u_1$ ($u_0 < -u_1$). Once the crack tip location is known, cohesive zone which is treated as a representative of an extended crack tip, can then be identified. Therefore, unless the crack propagation path is well known a priori under a prescribed loading conditions, it is essential to locate the crack tip at every simulation time step at which the data is acquired in order to correctly identify group of atoms constituting cohesive zone. We note that this task of identifying cohesive zones is relatively simple if the crack propagation path is known at the beginning of the simulation. In this case, such group of atoms at every time-step can be identified right at the start. However, in case of non-planar crack propagation, which usually occurs when the specimen with a crack is subjected to mixed-mode loading, cohesive zones need to be identified dynamically by first identifying the location of the crack-tip at every time-step relevant to data extraction. Note that this is true even in all cases of interfacial debonding in a bi-material as discussed in the previous section. Planar crack extension primarily occur if the specimen is subjected to mode-I tensile loading conditions, and most of the work focusing on determining CZ modeling parameters consider this type of loading condition alone.

Traditional approach to determine cohesive zones ahead of the crack tip using atomistic simulations is illustrated in the left diagram of Fig. 2. Fig. 2 shows a schematic of a bi-crystal with a (001) type STGB interface containing an intergranular crack. Snap-shots shown toward left and right side of the figure presents two different scenarios. First scenario on the left (traditional approach) presents series of snap-shots of region near the tip of a propagating crack at every $t_1 \Delta t$ time-step. Here $t_1$ is a positive integer and $\Delta t$ is the simulation time-step (generally chosen to be 1–3 fs). Note that this case presents planar inter-granular crack growth – typical response displayed by a cracked specimen under mode-I tensile loading. Hence, the crack propagation path is known a priori i.e. along the GB interface. Therefore, all regions constituting cohesive zones, comprising of groups of atoms along and in the vicinity of the GB interface, can be determined right at the beginning of the simulation. Yamakov et al. (2006) introduced an approach which allows mapping of collective mechanical response of such groups of atoms to the response of the cohesive zones at continuum scale. The general framework is adopted by many researchers since its introduction. First, a horizontal layer is defined, centered around the crack plane, of height of $2b_0$ (see first frame of the diagram on the left of Fig. 2) extending to $\pm h$, on both sides of the interface. This layer is further divided into regions with width $\delta_x$ (both $\delta_x$ and $\delta_y$ are few nanometers). This results in several cuboidal regions (see the shaded regions in schematic on the left) of $\delta_x \times 2b_0 \times t$ dimension ($t$ is the specimen thickness) which serve as cohesive zones as crack propagates through them. Subsequently, data is extracted from these regions every $n_1 \Delta t$ time-step. Mechanical response of groups of atoms in each region is used to obtain traction–displacement data during the course of steady state crack propagation characterizing cohesive zone model at the continuum scale (for further details refer to the work of Yamakov et al. (2006)).

This simplified approach, however, cannot be used to identify desired groups of atoms, used to construct cohesive zones if the crack growth is non-planar. An example of such scenario is presented by virtue of series of snap-shots in Fig. 2 on the right which is a typical response of a cracked specimen under mixed-mode loading. Note that as crack deflects and grows out-of-plane, the group of atoms (say at step time $t = t_1 + n_1 \Delta t$ and shown as series of shaded regions in the second frame on right in Fig. 2) constituting the cohesive zones, are no longer the ones constituting the GB interface at beginning of the simulation (at step-time $t = t_1$ shown as shaded regions in the first frame). Atomic regions determined at these two time-steps, $t = t_1$ and $t = t_1 + n_1 \Delta t$, as shown in grey shades in the figure are different from each other. This phenomenon, apparently, continues at later time steps as well and is illustrated clearly in the third and fourth frame. This clearly indicates that in such cases atomic regions ahead of the crack tip constituting cohesive zones can only be determined at current time-step and are different from those determined in the previous time steps. Determination of such regions require identification of the crack-tip location at every time-step of interest. For example, in first frame on the right in Fig. 2, once the crack tip location is determined, group of atoms constituting a region of dimension $\delta_x \times 2b_0 \times t$ can also be determined at time $t_1$ as illustrated in grey shade just near the crack-tip. We note that the average potential energy of the group of atoms in this region is lower than those constituting atoms on the surface. As the crack propagates, such regions are subsequently determined dynamically at every $n_1 \Delta t$ time-step. We denote such regions as parent regions; examples of parent regions $R_1, R_2, R_3, ..., R_n$ can be seen in the schematic in Fig. 2 at $t_1 + n_1 \Delta t, t_1 + 2n_1 \Delta t, t_1 + 3n_1 \Delta t, t_1 + 2n_1 \Delta t, t_1 + 3n_1 \Delta t, ..., t_1 + (n - 1)n_1 \Delta t$ times, respectively. Traction–separation data is recorded from these parent regions at each $n_1 \Delta t$ time-step. Although, new regions are dynamically determined as the crack propagates, traction–separation history data from group of atoms constituting older regions, determined at previous time-steps, are also monitored. These other regions $R_{1,1}, R_{1,2}, R_{2,1}, ..., R_{n-1,4}$ as specified in the schematic in Fig. 2, stem from parent regions from previous time-steps. For example, $R_{1,1}, R_{1,2}$, etc. constitutes same atoms which formed parent Region $R_1$; state of these regions represents history of the cohesive zone $R_1$ from its inception at time $t = t_1$ (i.e. beginning of inelastic deformation in that region at time $t = t_1$) all the way to complete decohesion.

3. Results and discussions

3.1. Stress–strain response and crack propagation

Fig. 3(a) & (b) present plots of average (global) tensile and shear stress/strain response, respectively under various mixed-mode
loading conditions and the maximum simulation time was considered to be about 1.2 ns. Global stresses shown in the plots were computed using the virial theorem (Subramaniyan and Sun, 2008) and corresponding engineering strains were obtained from the boundary displacement in the normal and shear directions (for tensile and shear strain, respectively). Values of displacement, strain and stress were averaged over 10 time-steps before plotting. Note that it is evident from these plots that as the shear component of the mixed-mode loading increases (i.e. with the increase of $\theta$ characterizing mode-mixity (see Table 1)), overall strain-to-failure also increases. In this type of bicrystalline specimen with $\Sigma 5$ (210)$\langle 001 \rangle$ STGB interface, three types of energy dissipative mechanisms characterize inelastic deformation – shear coupled GB migration away from the crack-tips, change in spacial orientation of GB structural units rendering highly disordered grain boundary near the crack tips and brittle intergranular fracture. Loading mode-mixity determines the dominant deformation mechanism and the effects are manifested on the stress–strain response at various $\theta$. Activation and interplay of these three deformation mechanisms can be explained by considering an example of a case when the specimen is subjected to a shear dominant loading with $\theta = 75^\circ$. Fig. 4 presents the snap-shots of the specimen undergoing deformation at times 350, 450 and 610 ps; stress–strain state of the specimen at these times is also identified in tensile and shear stress–strain plots in Fig. 3(a) and (b) by points 1, 2 and 3, respectively. Due to shear loading normal to the tilt axis in the GB plane, shear coupled GB migration is activated but at the same time, this migration is somewhat hindered due to the presence of intergranular crack. The crack pins the GB near its tips causing it to bulge out, and the shear coupled migration (SCM) primarily occurs ahead of this region which is affected due to GB pinning (i.e. regions both, on the right and on the left of the crack tips). The sheared zone due to SCM along with the grain boundary structural units after migration are identified in Frame-1 (and similarly in other two frames) of Fig. 4 and also in the inset which display atoms not in the FCC coordination. Frame-1 shows that both crack-tips pin the grain boundary interface, as a result of which it becomes non-planar. This causes the crack-kinking from the crack-tip on the left, where as crack-tip on the right remains dormant. Atoms constituting this region near the crack-tip on the right are thereby in a highly disordered state which subsequently hinders crack initiation from that tip. Crack do not initiate from this tip throughout the simulation and spatial orientation of atoms in the vicinity of this tip, particularly along the interface, becomes dif-
different and random compared with the GB structural units or with those atoms in FCC coordination. This ‘atomic-disorder’ becomes more prevalent, grows and increase in size as the GB migrates upon continued loading as seen in Frame-2. Meanwhile, crack kinks out of the interface from the left tip and grows in a non-planar fashion as SCM of the STGB continues accompanied by growing shear-zone as seen in Frame-2. Therefore, all three mechanisms described above constitute inelastic deformation at times between frames 1 & 2. Corresponding to times between frames 1 and 2, points 1 and 2 in Fig. 3(a) and (b) show tensile stress growth with increasing tensile strain is significantly retarded and overall shear stress drops with the increase in the shear strain. On the other hand, at times between frames 2 & 3, faster crack propagation somewhat parallel to the GB interface seems to dominate the energy dissipative deformation mechanism. Frame-3 shows that crack-propagation is the dominant mechanism compared with increase in atomic-disorder or SCM. Signature of this inelastic mechanism is quite clear on the stress–strain curve (as shown by points 2 and 3), where both tensile and shear stresses drops significantly with the increase in their respective strains.

Note that one of the distinctive feature which differentiate shear stress–strain curves with their tensile stress–strain counterparts for all mixed-mode conditions is the stress-drop & -rise interspersed between stages of overall stress evolution with the increase in the shear strain. This shear stress-drop & -rise is a typical characteristic of the shear stress behavior during SCM and has been reported before for several (001) type STGBs in Cu bicrystal in the presence of nano-cracks and precipitates along the GB interface (Luque et al., 2009). In the absence of intergranular crack when SCM of the grain boundary is the strain accommodative mechanism alone, it is reported in various studies that shear stress displays stick–slip type of behavior akin to sliding friction (cf. Cahn et al., 2006a; Sansoz and Molinari, 2005). Therefore, this stress-drop & -rise feature apparently becomes more prominent in the shear stress–strain curves as mode-mixity $\theta$ increases from 0° to 85° i.e. as the contribution of SCM of STGB to inelastic deformation increases, and due to crack propagation decreases. This feature is also underscored in Fig. 5 which characterize crack propagation. Fig. 5 presents the $x$- and $y$-coordinate of the crack tip (on the left of the specimen) normalized by the length and the height of the box, respectively vs. time. Note that the first thing which the figure shows is that the rate of crack growth or the crack speed decreases with the increase in the mode-mixity. Secondly, the crack growth becomes increasingly non-planar with the increase in mode-mixity as is evident from higher values of the normalized $y$-coordinates of the crack tip at higher mode-mixity values for a given normalized $x$-coordinate of the tip; $y = 0$ is the crack tip position along $y$-axis at the beginning of the simulation. The reason is, with the increase in the mode-mixity, shear component of overall loading which drives shear coupled GB migration also increases. This in-turn results in crack propagation becoming less prevalent dissipative mechanism compared with SCM. For example, at $\theta = 85^\circ$ at time of 1.5 ns due to significant SCM of the grain boundary, the crack propagated barely half-way across the length of the specimen and yet it is near the horizontal boundary at the bottom as is evident from its tip's normalized $x$- and $y$-coordinates, respectively. On the other hand, due to lack of significant SCM at $\theta = 45^\circ$, normalized $x$- and $y$-coordinate of the crack tip, respectively, suggest that within about just 0.26 ns, crack has propagated across the boundary and that out-of-plane growth during those times have been relatively less. This is a clear indication of mode-mixity dependent inelastic and failure mechanism in this bicrystal. Note that this is in stark contrast with earlier studies on several bimaterial systems subjected to mixed-mode loading as described in the introduction section. For example, unlike the present case, in the study presented by Zhou et al. (2009) on a brittle BCC type of bicrystalline system, mode-mixity did not have profound influence on their in-plane crack growth dynamics as planar brittle intergranular fracture was the only dominant dissipative mechanism independent of mode-mixity; this is similar in other studies as well discussed in the introduction section. For $\theta = 75^\circ$, the state of the specimen, depicted in frames 1, 2, 3 in Fig. 4 is identified on the crack growth curve as well, as shown

![Figure 5](image-url) Fig. 5. Figure presents the plots of the $x$- and $y$-coordinate of the crack tip (on the left of the specimen) normalized by the length and the height of the box, respectively vs. time.
by points 1, 2, 3, respectively in Fig. 5. This crack propagation mechanism is in excellent correlation with changes depicted in the tensile & shear stress–strain curves in Fig. 3(a) and (b) by points 1, 2 and 3. It is quite clear from the crack propagation plot for $\theta = 75^\circ$ that as the dominating deformation mechanism is crack growth compared with the SCM or due to increase in the atomic disorder, the crack growth at times between frames 2 & 3 is considerably faster than at times between frames 1 & 2. Correspondingly, the tensile and shear-stress drop significantly at times between frames 2 & 3, as shown by markings in Fig. 3, compared with the stress states at times between frames 1 & 2.

3.2. Localized traction–separation law

Localized normal and shear tractions in the vicinity of the growing crack and corresponding crack-opening-displacement are required to characterize the cohesive zone law. In order to obtain such local traction–separation values, cohesive zones are first determined at every time step of interest after the crack initiation for various mixed-mode loading conditions considered in this work. Crack propagation curves shown in Fig. 5 suggest that the crack acquires a reasonable steady state propagation state once it is initiated. Although we note that as SCM becomes increasingly dominant deformation mechanism with the increase in loading mode-mixity $\theta$, the propagation becomes increasingly discontinuous with time as $\theta$ increases to 75° and 85°. In the present study, determination of the cohesive zones and computation of tractions and crack opening displacements are performed at every 0.5 ps after the crack initiation. Figs. 4 and 5 also suggest that in this bcc-crystalline system, the crack growth becomes increasingly non-planar as the shear component or the mode-mixity of the loading increases. Therefore, as described in Section 2, the determination of cohesive zones at all times during the deformation cannot be made a priori; they are determined at every time-step of interest as the system continues to deform. To determine these cohesive zones at every 0.5 ps, following groups of atoms are determined first – atoms lying on fully separated surfaces, atoms constituting the GB structural units, and atoms in the disordered state – along with all other atoms which are within the distance of 5 Å to these groups of atoms. These groups of atoms change more often during times when the SCM dominates the deformation mechanism, an example of which is presented later in this section. Next, this group is divided into regions of width $\Delta x$ which was chosen to be 10 Å in this study. Subsequently, the crack tip is located which finally leads to the identification of the cohesive zone at that time-step. These cohesive-zone regions are called the parent regions. Normal and shear tractions at a local position (i.e. $x$-coordinate defined by the centroid of the parent region) are computed as the average atomic stresses of all atoms in that region, and the normal and shear components of the crack opening displacement, $\Delta x$ and $\Delta y$, are calculated as the corresponding components of the average atom displacement in the upper half of the region with respect to that of the lower half (upper and lower halves were identified $s$ regions above and below the centroid, respectively). The total magnitude of the crack opening is defined as $\Delta r = \sqrt{\left(\Delta x\right)^2 + \left(\Delta y\right)^2}$; all these values e.g. centroid, tractions, crack-opening-displacements are averaged over 10 time-steps and are centered over the time of output. Although new parent cohesive-zone regions are determined at every 0.5 ps, history of the deformation of older parent regions including the evolution of their shear & normal tractions and crack-opening-displacement are also recorded for 20 ps. During this time for every mixed-mode loading conditions, each parent region transforms from being in a fully intact state to a complete damaged state; an example below provides more description on this transformation.

Fig. 6(a) and (b) illustrate the parent cohesive zone regions identified at 566 ps and at 580 ps, respectively. Both figures show three snap shots each, of the portion of the specimen near the GB interface subjected to mixed-mode loading of $\theta = 75^\circ$. First frame, on the top of Fig. 6(a) (and similarly, of Fig. 6(b)) shows the state of the specimen on the left, followed by the group of atoms identified along and in the vicinity of the cracked surface and the interface, and finally, plots of spatial distribution of the normal and shear stresses on the right. The inset of the highlighted region, in the first frame of both Fig. 6(a) and (b), shows the magnified view of the parent cohesive-zone region determined at those time steps. Note that the tensile stress at the location of the parent cohesive-zone region is maximum and the shear stress is close to its maximum value. Next two frames in both Fig. 6(a) and (b) show the history of the deformation of the group of atoms identified at 566 and 580 ps, respectively. The change in the normal and shear stress distribution is also shown alongside; the inset in both figures show the deformation history of the parent cohesive-zone region at times specified in the respective frames. Fig. 6(a) and (b) apparently present two contrasting dominant deformation mechanisms which are evident from the deformation history of their respective group of atoms and their parent cohesive-zone region. Fig. 6(a) shows that SCM of the STGB is the strain accommodative dominant mechanism from 566 to 580 ps; thereafter, from 580 to 583 ps, crack propagation takes over as dominant mechanism as shown in Fig. 6(b). During 566 to 580 ps, crack extension becomes largely non-planar due to SCM and, therefore, the parent cohesive-zone region determined at 580 ps (shown in the inset in the first frame of Fig. 6(b)) is composed of different atoms than those determined at 566 ps (shown in the inset of first frame of Fig. 6(a)). Note the group of atoms at 580 ps shown in the third frame of Fig. 6(a) is different from those at 580 ps shown in the first frame of Fig. 6(a). Both figures also display the intact, partially damaged and final separation states of their parent cohesive-zone regions accompanied by their respective normal and shear traction which drops from near maximum to near zero as the damage progresses. Note that the damage progression from intact to fully separated parent regions is faster as expected (within about 3 ps) when crack propagation is the dominating mechanism (see Fig. 6(b)) as opposed to slower progression (within about 14 ps) when stain accommodative SCM is more dominant (see Fig. 6(b)). Fig. 7(a) and (b) present the time evolution of the spatial distribution of the potential energy of group of atoms, around the cracked surfaces and the interface identified at 566 and 580 ps, respectively (second image on the top frame of Fig. 6(a) and (b) shows the group of atoms at 566 and 580 ps, respectively). Each energy vs. $x$-coordinate curve in Fig. 6(a) and (b) is 2 and 0.5 ps apart, respectively. Therefore, it can be clearly deduced from the plots that formation of fully fractured surfaces took longer at 566 ps when SCM was the strain accommodative dominant deformation mechanism as compared with the time at 580 ps when crack propagation dominated the deformation causing the potential energy to rise from $\sim 3.475$ to $\sim 3.36$ eV.

3.3. Formulating cohesive zone model

Both normal and shear traction vs. separation (or crack-opening-displacement) data were computed from several locations and times during crack propagation for seven mixed-mode loading conditions (see Table 1). The separation data points, paired with corresponding traction data points, were sorted in the ascending order and then were binned with a bin size of 0.1 Å. The average values of traction and separation corresponding to a bin were subsequently obtained by computing the mean of every traction and separation data point, respectively, in that bin. Fig. 8 shows the plots of normal and shear tractions vs. separation for various
mixed-mode loading conditions. Note that all plots display general trends expected from most traction–displacement curves i.e. the stress (traction) initially rises with the increase in separation (displacement) and reaches a maximum, then decreases and goes to zero as the faces are completely separated. We denote the peak stress as $\sigma_{\text{max}}$ and the displacement corresponding to $\sigma_{\text{max}}$ as $\delta_{\text{0}}$; displacement at which the stress goes to zero is denoted as $\delta_{\text{max}}$.

It is also noted that as the shear component of the loading increases, the decay of both tensile and shear stresses after the peak stress is not as rapid with the increase in separation, particularly for $\theta = 75^\circ$ and $85^\circ$ compared with lower values of $\theta$. This results in higher $\delta_{\text{max}}$ as the mode-mixity increases; the effect is stronger for $\theta = 75^\circ$ and $85^\circ$. Apparently, SCM becomes increasingly dominant deformation mechanism as $\theta$ approaches $85^\circ$, resulting in
Fig. 7. Figure presents the time evolution of the spatial distribution of the potential energy of group of atoms, around the cracked surfaces and the interface identified at (a) 566 ps and (b) 580 ps, respectively.

Fig. 8. Series of plots showing the tractions (both tensile and shear) as a function of crack opening displacement and corresponding fitting curves for various mode-mixity.
slower crack propagation rate. This further results in slower damage evolution (from being in an intact state to partially ruptured state, finally leading to complete decohesion) in a cohesive zone which, therefore, can sustain higher deformation as discussed in previous section and demonstrated in Fig. 6(a) and (b). At lower $\theta$, brittle crack propagation is the dominant energy dissipative mechanism which result in both, relatively faster damage evolution and lower deformation at which the load carrying capacity
of a cohesive zone drops to zero. Response of cohesive zones as a result of these deformation mechanisms are manifested in series of traction–separation curves shown in Fig. 8.

For each macroscopic mixed-mode loading state, average local mode-mixity experienced by the cohesive zones is also computed. Local mode-mixity can be defined as

$$\phi = \sin^{-1} \frac{\Delta y}{\sqrt{\Delta x^2 + \Delta y^2}}$$

where $\Delta x$ and $\Delta y$ are the shear and normal crack-opening-displacement in the cohesive zones, respectively. The local mode-mixity angle $\phi$ measures the relative shear displacement with respect to the overall crack-separation in a cohesive zone as opposed to $\theta$ which describes the shear component of the overall global loading. The average value $\phi^m$, computed as a mean value of $\phi$ obtained from every cohesive zone in a simulation, is considered to be better suited to characterize the localized mixed-mode conditions prevailing during the deformation of the cohesive zone. This computed average value is within a few degrees to its corresponding value of $\theta$ and equals $2.3^\circ$, $20.1^\circ$, $36.3^\circ$, $52.4^\circ$, $65.6^\circ$, $75.8^\circ$, $81.5^\circ$ for $\theta = 0^\circ$, $15^\circ$, $30^\circ$, $45^\circ$, $60^\circ$, $75^\circ$, $85^\circ$, respectively. Considering the traction–separation data from each MD simulation, both shear and normal traction can be expressed as a function of crack-opening-displacement $\Delta r$, using the following function

$$\sigma = \frac{\sigma_{\text{max}}}{\delta_0} \Delta r \exp \left[ \left\{ 1 - \frac{(\Delta r/\delta_0)^2}{d} \right\} / d \right]$$

Table 2

<table>
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<th>Cohesive zone model parameters.</th>
<th>$a_0$</th>
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<th>$a_2$</th>
<th>$a_3$</th>
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<tr>
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<td>$d$</td>
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<td>-7.108</td>
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Fig. 10. Surface plot of (a) normal, and (b) shear stress as a function of mode-mixity and crack opening displacement.
In this equation, parameters $\sigma_{\text{max}}$ is the maximum stress, $\delta_0$ is the corresponding displacement and $d$ controls the overall shape and the rate of decay of the stress with the increase in displacement. We note that this cohesive zone law bears strong resemblance with another more popular and robust law introduced by Needleman (1988) to characterize interfacial debonding; we use an additional shape parameter $d$ (which was not used in their model) as it helps in achieving a better fit to the data. These three parameters $\sigma_{\text{max}}, \delta_0$ and $d$ separately characterizing normal and shear traction/ separation laws, are obtained for all seven cases with different mixed-mode loading conditions, and are expressed as a function of local mode-mixity angle $\phi^m$. This implies that once the local mode-mixity is known, all these parameters can also be determined. Fig. 9(a) through (f) presents plots of these parameters (for both normal and shear traction–displacement cohesive zone law) as a function of $\phi^m$. Considering the variation of these parameters with the mode-mixity as presented in the plots, the following functional forms are utilized to fit the data.

$$F_1 = a_0 + a_1 \phi^m + a_2 (\phi^m)^2 + a_3 (\phi^m)^3$$

$$F_2 = a_0 (\phi^m)^n + a_2$$

Functional form $F_1$ is used to describe the variation of $\sigma_{\text{max}}$ and $d$ with $\phi^m$, and functional form $F_2$ describes the variation of $\delta_0$ with $\phi^m$. The parameters used to fit these functions are provided in Table 2. Results from these parameterized functions are in good agreement with the results obtained from several MD simulations as shown in Fig. 9. Using these results, a complete 3-D shear and normal tractions as a function of crack opening displacement and mode-mixity are computed. These results in the form of surface plots are presented in Fig. 10. Note that two important features can be inferred from the figure – Fig. 9(a) and (b) shows that as mode-mixity increases, both $\delta_0$ and separation-to-complete-debonding ($\delta_{\text{max}}$) increases, and Fig. 9(b) shows that pure shear loading (i.e. $\phi^m = 90^\circ$) can result in both tensile and shear traction. These features in CZM surface plots are direct results of the dominant mechanisms activated with the increase in mode-mixity, i.e. as $\phi^m$ increases, there is significant SCM of the grain boundary along with high degree of atomic-disorder near the crack tip. This leads to mixed-mode stress state even under predominant shear loading along with an increase of both $\delta_0$ and $\delta_{\text{max}}$.

Fig. 11 shows the plots of work of separation due to tensile and shear loading as a function of mode mixity $\phi^m$. The work of crack separation is computed by integrating CZM traction–displacement curves (Eq. (1)) as a function of mode-mixity $\phi^m$. Figure suggests that the total work of separation curve displays slight oscillation where it remains somewhat constant at about $5J/m^2$ as $\phi^m$ increases from $0^\circ$ to $10^\circ$ after which it decreases to $2.5J/m^2$ at $\phi^m = 45^\circ$ and then increases to $7.2J/m^2$ as $\phi^m$ approaches $90^\circ$. The trend of all the plots are similar to those presented by Zhou et al. (2008,2009). The work of adhesion for the present case of bicrystal Cu is defined as $2\gamma_{(210)-\gamma_{(200)}(0\bar{1}0)}\gamma_{(200)}$ where $\gamma_{(210)}$ is the Cu (210) surface energy and $\gamma_{(200)}$ (2 0 0) is the $\Sigma 5 (210)/[001]$ STGB interface energy. Work of adhesion is computed as $2 \times 1.6175 \times 1.0597 = 2.1753 J/m^2$. Note that unlike work of adhesion (which is constant) work of crack separation is a function of the mode-mixity $\phi^m$ and is higher than work of adhesion; similar observations have been made for various brittle and ductile interfaces e.g. Figure 13 by Zhou et al. (2008), Figure 13 by Yamakov et al. (2006).

### 4. Summary

An improved and novel methodology is developed using atomistic simulations and cohesive zone modeling to characterize interfacial debonding subjected to general mixed-mode loading conditions. Unlike models developed previously by several authors, present framework does not assume the crack path apriori directed along the undeformed interface configuration. It explicitly accounts for non-planar propagation – situations pertaining to most realistic interfacial debonding of large class of material systems particularly under mixed-mode loading- and dynamically determines the cohesive zones during the crack propagation. Once the cohesive zones are determined at various stages of crack propagation, their traction and crack-opening-displacement (COD) values are recorded from these parent regions. Although, new regions are dynamically determined as the crack propagates, traction – COD history data from earlier cohesive-zone (determined at previous time-steps) is also recorded allowing the monitoring of the inception of inelastic deformation all the way to complete decohesion. This methodology is applied to study the interfacial fracture of a Cu bicrystal with a $\Sigma 5 (210)/[001]$ symmetric tilt grain boundary interface subjected to several mixed-mode loading conditions. In the presence of intergranular crack, three types of energy dissipative mechanisms characterize inelastic deformation in this bicrystalline specimen – shear coupled GB migration away from the crack-tips, change in spacial orientation of GB structural units rendering highly disordered grain boundary near the crack tips and brittle intergranular fracture. Mode-mixity of the loading determines which combination of these three deformation mechanism will be active at various stages of loading. It is observed that as mode-mixity increases, ratio of the shear component of overall loading which drives shear coupled GB migration compared with the normal loading also increases which in-turn results in crack propagation becoming less prevalent dissipative mechanism compared with shear coupled migration. Furthermore, the resulting crack growth becomes increasingly non-planar and the determination of cohesive zones at all times during the deformation cannot be made apriori as was the case with previous models. Using statistics of the data obtained for several mixed-mode loading conditions, traction–displacement curves characterizing interfacial debonding are obtained. These curves demonstrates that as SCM becomes a dominant deformation mechanisms at higher mode-mixity, the propensity of the cohesive zone to bear
the load at higher deformation also increases. On the other hand, lower mode-mixity loading (when the brittle crack propagation is the dominant damage mechanism) results in relatively faster damage evolution and lower deformation at which the load carrying capacity of a cohesive zone drops to zero. In order to fit the traction–displacement data at various mode-mixity, a modified version of the exponential law introduced by Needleman (1988) is used to describe both shear and normal traction as a function of crack-opening-displacement. The parameters of the cohesive law were further expressed as a function of the mode-mixity and a complete 3-D shear and normal tractions as a function of crack opening displacement and mode-mixity are computed.

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