

MULTISCALE MODELING OF DAMAGE PROCESSES IN fcc ALUMINUM: FROM ATOMS TO GRAINS

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Abstract

Molecular dynamics (MD) methods are opening new opportunities for simulating the fundamental processes of material behavior at the atomistic level. However, current analysis is limited to small domains and increasing the size of the MD domain quickly presents intractable computational demands. A preferred approach to surmount this computational limitation has been to combine continuum mechanics-based modeling procedures, such as the finite element method (FEM), with MD analyses thereby reducing the region of atomic scale refinement. Such multiscale modeling strategies can be divided into two broad classifications: concurrent multiscale methods that directly incorporate an atomistic domain within a continuum domain and sequential multiscale methods that extract an averaged response from the atomistic simulation for later use as a constitutive model in a continuum analysis.

In the present work, new approaches to both concurrent and sequential multiscale modeling are developed. A new approach to concurrent MD-FEM coupling uses statistical averaging of the atomistic MD domain to provide displacement interface boundary conditions to the surrounding continuum FEM domain, which, in return, generates interface reaction forces applied as piecewise constant traction boundary conditions to the MD region. Additionally, a new approach to sequential multiscale modeling is developed and based on the definition of a cohesive zone volume element (CZVE). The CZVE is an atomistic analog to the cohesive zone models that are often used to model material degradation in continuum finite element analyses. Taken together, these two approaches are an attempt to recast atomistic processes within a format suitable for inclusion in grain-scale finite element analyses and are providing a necessary step toward true physics-based analysis of damage processes.

I. Introduction

Classical fracture mechanics is based on the comparison of computed fracture parameters to their empirically-determined critical values. Although this paradigm has been extremely

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successful for modeling crack growth at structural scales, it does not describe the physical processes that govern fracture. Ultimately, the characterization of events and processes that occur at length scales on the order of 10^{-9} to 10^{-3} m is needed to *understand* the physics of crack growth.

Physics-based modeling of fracture begins at nanometer length scales in which atomistic simulation is used to predict the formation, propagation, and interaction of fundamental damage mechanisms. These mechanisms include dislocation formation and interaction, interstitial void formation, and atomic diffusion. These nanoscale damage mechanisms progress into microscale processes such as local plasticity and small crack formation. Ultimately, damage progression leads to macroscopic failure.

However, modeling atomistic processes quickly becomes computationally intractable as the system size increases. With current computer technology, the computational demands of modeling suitable domain sizes (on the order of hundreds of atoms for quantum mechanics-based methods, and potentially billions of atoms for classical mechanics-based methods) and integrating the governing equations of state over sufficiently long time intervals quickly reaches an upper bound for practical analyses. In contrast, continuum mechanics methods such as the finite element method (FEM) provide an economical numerical representation of material behavior at length scales in which continuum assumptions are appropriate. Thus, multiscale modeling strategies are needed that use the most efficient material model at each length scale to develop a unified description of the hierarchy of processes that govern fracture.

Multiscale modeling strategies relevant to length scales between the atomic-scale and the lower end of the grain-scale can be divided into two broad classifications: concurrent multiscale and sequential multiscale. Concurrent multiscale modeling bridges length scales by coupling different computational paradigms and is attractive as a highly efficient means of reducing the computational cost of the simulations in cases that require modeling of relatively large material domains to capture the complete deformation field, but where atomic and subatomic refinement is needed only in very localized regions (e.g., near a crack tip or dislocation core). Such computational issues arise in modeling crack nucleation and propagation, and in modeling dislocation formation and interaction. Concurrent multiscale models allow the size limitations of the atomistic simulation to be avoided by embedding an inner MD region (where complex dynamic processes and large deformation gradients exist) within an outer domain (where small deformation gradients exist) where a continuum representation of the material becomes appropriate.

In contrast, sequential multiscale modeling relies on recasting previously developed characterizations of damage processes as constitutive models within higher-level analyses. Cohesive zone models have often been used as a means of sequential multiscale modeling by developing an interfacial traction-displacement relationship using bulk material properties to model possible fracture surfaces in a continuum.¹⁻⁵ The use of cohesive zone models in finite elements permits highly discontinuous displacement behavior to be exhibited in a single discretized model without remeshing while using an incremental piecewise linear solution algorithm.

In this paper, elements of both concurrent and sequential multiscale modeling will be used to illustrate the possibilities of characterizing fracture along grain boundaries in polycrystalline aluminum. An outline of a new concurrent multiscale method for coupling MD and FEM computational domains is presented in Section II. Section III summarizes the determination of cohesive zone relationships developed from molecular dynamics analysis using a new sequential multiscale modeling method. Also in Section III is a discussion of a simulation of an edge crack propagating through a continuum into an atomistic domain with the deformation along the crack plane in the continuum region modeled using CZMs. Section IV presents a simulation of intergranular fracture in a polycrystal where the CZMs are used as constitutive models along idealized grain boundaries. Finally, Section V presents a summary of the analysis and overall methodology.

II. Concurrent Multiscale Modeling

Over the past decade, various methods that directly couple material representations at different levels of refinement have been developed and offer significant computational advantages compared to full atomistic simulations for predicting deformation and fracture processes.⁶⁻¹⁶ A common feature of all of these approaches for coupling atomistic regions with continuum domains is the refinement of the FEM mesh to the atomic scale. While such direct coupling approaches are conceptually straightforward, the fundamental difficulty in their development lies in the inherent differences between the atomistic and continuum computational models. The physical state of the atomistic region is described through nonlocal interatomic forces between discrete atoms of given position and momentum, while the physical state of the continuum region is described through continuous stress-strain fields that reflect local statistical averages of atomic interactions at larger length and time scales.

However, a robust connection between continuum and discrete quantities can be achieved through a statistical averaging over length and time scales where the discreteness of the atomic structure can be successfully approximated as a continuum. With the use of statistical averages to couple the two computational schemes, the developed approach constitutes a *statistical* coupling approach, and the developed MD-FEM coupling method is referred to as the embedded statistical coupling method (ESCM).^{17,18} The resulting model that consists of an MD system embedded in a FEM domain is depicted in Figure 1.

The structure of the basic ESCM model consists of four regions that are depicted in Figure 2. The regions include the inner MD region, interface MD/FEM region, surface MD region and FEM domain. The inner MD region is used to model the damage processes (e.g., plastic deformation events such as dislocation or void nucleation, crack propagation) that evolve during the simulation. The interface MD/FEM region provides the computational linkage between statistical averages of atomistic quantities from the MD and continuum forces and displacements from the FEM. The surface MD region does not interact with superposed FEM nodes but, rather, is used to compensate for atomic free edge effects at the outer boundary of the MD region. Finally, the FEM domain permits a large reduction in the computational cost of the simulations by replacing the atomistic representation with a continuum model in those regions of the system

where the deformation gradients are small and atomic-level resolution is not necessary. Complete details of the basic method are presented by Saether et al.^{17, 18}

The basic algorithm of ESCM involves the statistical averaging over both time and volume of atomistic subdomains at the MD-FEM interface that provide nodal displacement boundary conditions to the continuum FEM domain. An analysis of the FEM domain is performed, which, in turn, generates interface reaction forces that are applied as constant traction boundary conditions¹⁹ to the atoms within the localized MD subdomain. The MD system is simulated to accommodate the interface reaction forces and to provide an update of the displacement boundary conditions at the MD-FEM interface. This process is iterated until equilibrium between the atomistic MD forces and the FEM reaction forces is established at the interface. Typically, one finite element at the interface encompasses a region of several hundred to several thousand atoms. At this scale, the discreteness of the atomic structure is homogenized enough so that the FEM domain responds to the atomistic domain as an extension of the continuum.

A recent addition to the ESCM involves the addition of cohesive zone model (CZM) elements along the crack plane to improve the compatibility of the deformations near the MD to FEM interface. Cohesive zone models approximate debonding processes along an interface^{1-5, 20} and are frequently used in conjunction with finite element approaches to study fracture in a wide variety of materials. Recently, cohesive zone volume elements (CZVEs)²¹ have been introduced in the MD analysis to calculate atomistic-based parameters defining CZMs. The resulting CZMs exhibit the aggregate behavior of a volume of atoms in the MD simulation.²¹ By placing the CZM elements along the plane of crack growth within the finite element domain of the ESCM model, the fracture process can be simulated in the continuum as the crack approaches the MD-FE interface. Figure 3 depicts the coupled MD-FEM model containing an edge crack. CZM elements are identified that represent the cohesive properties of the grain boundary (GB) in the continuum. Crystal I and crystal II identify the MD regions that have been rotated through a tilt angle to form the GB. The CZVEs will be discussed in more detail in the Section III.

The simulation presented in this paper considers intergranular fracture wherein MD simulations of fracture along grain boundaries (GBs) are used to obtain the atomistic response of crack propagation under applied loads along a characteristic length of the GB. Intergranular, rather than transgranular, fracture is considered because the crack path is well-defined and is known a-priori.

Figure 4 shows a $\langle 110 \rangle$ $\Sigma 99$ symmetric tilt GB, a typical high energy GB formed between two grains in a fcc metal. Because of the slip plane orientation near this GB, crack growth in the $+x$ direction was observed to be brittle with few dislocations emitted, while crack growth in the $-x$ direction was observed to be ductile with many dislocations and twins emitted.²¹ Common neighbor analysis (CNA)^{22, 23} is used to identify atoms in different crystallographic states: fcc (small dots), hcp (triangles), non-crystalline atoms (large dots), and surface atoms (squares), indicating existing vacancies in the GB. The length scale is in units of the lattice constant of Al, $a_o = 0.405$ nm, and the analysis is performed using the potential of Mishin and Farkas.²⁴

III. Sequential Multiscale Modeling

Development of Traction-Displacement Relationships from MD

Through the definition of CZVEs shown in Figure 5, the results from MD simulations have been recast to obtain averaged continuum traction-displacement relationships that represent the cohesive interactions along a characteristic length of material. Using a purely MD model of a center crack along the $\Sigma 99$ grain boundary presented in Reference 21, the stress and opening profiles are extracted along the crack growing in the system as shown in Figure 6. The figure shows distinct traction, $\sigma_{yy}(x)$, and displacement, λ , profiles for the two crack tips of the center crack. The asymmetric behavior results from the orientation of the crystal lattice of the grains forming the grain boundary. A curve fit of $x^{-1/2}$ in Figure 6 is shown as a close approximation to the $\sigma_{yy}(x)$ values extracted from the MD for the brittle tip. In contrast, plastic deformation processes, including twinning and dislocation emission, were found to dominate deformation at the ductile crack tip growing in the opposite direction.²¹

The $\sigma_{yy}(x)$ and $\lambda(x)$ profiles in Figure 6 represent the traction and opening displacement at a single instant of time during crack propagation. If the entire simulation of the interface debonding is divided into N_t equal intervals of time t_q ($q \in [0, N_t]$), numerous similar profiles can be taken of many CZVEs placed along the GB. When plotted as a σ_{yy} vs. λ curve, each $(\sigma_{yy}(x_p, t_q), \lambda(x_p, t_q))$ pair represents a point $\sigma_{yy}(\lambda(x_p, t_q))$. After sorting these data points in order of ascending λ , so that $\lambda_i < \lambda_{i+1}$, and taking a moving average (or a consecutive mean),

$$\tau(\lambda_i) = \frac{1}{(2M+1)} \sum_{j=-M}^M \sigma_{yy}(\lambda_{i+j}) \quad (3)$$

in which the results are averaged over M points backward and M points forward from λ_i , a construction of a statistically representative cohesive zone relationship $\tau(\lambda)$ can be made. Complete details of the modeling, fracture processes, and extraction of the CZM response are given in Yamakov, et al.²¹

Crack Propagation through a Continuum-Atomistic Interface

A continuum-atomistic model for crack propagation in the brittle direction along the $\Sigma 99$ GB shown in Figure 3, and analyzed using the enhanced ESCM analysis, is presented. The dimensions of the coupled MD-FEM model used for this simulation are $d_{FE} = 900$ nm in the x - and y - directions, with a circular MD region in the x - y plane of diameter, $d_{MD} = 45$ nm, as shown in Figure 1. The system thickness in the z -direction is $h = 2.9$ nm with periodic boundary conditions to emulate a bulk atomic state in this direction. The simulation was performed at a temperature $T = 300$ K and maintained by a Nose-Hoover thermostat.²⁵

An edge crack was inserted along the line of symmetry, c , in the FEM mesh which ended with four finite elements on the left side before reaching the MD-FEM interface (Figure 3). These four remaining FEs were connected through CZM elements placed along the crack direction (line c in Figure 3), which meet the atomistic GB at the MD-FEM interface. On the

right side of the MD region, the debonding interface is continued through another line of CZM elements, which extends to the opposite outer boundary of the FEM domain.

The system was subjected to uniaxial far-field strain, ϵ_{yy} , applied as displacement boundary conditions at the outer boundary of the FEM domain. The strain was gradually increased from 0.4% to 2% in steps of 0.4% every 20 MD-FEM iterations (20 ps MD simulation time), allowing the MD system to more smoothly follow the stress increase in the surrounding FEM domain. The crack grows as an edge crack in the continuum environment subjected to mode I loading conditions and penetrates into the atomistic environment (Figure 7). The continuity of the crack propagation process through the MD-FEM interface is achieved by using the CZM constitutive relation derived for interface debonding based on the pure molecular-dynamics simulations²¹ as discussed previously. Figure 7 presents the system configuration and σ_{yy} stress state at the end of the second iteration when $\epsilon_{yy} = 2.0\%$.

The process of crack propagation is illustrated in Figure 8 through a set of snapshots, magnified to show the physical configuration of the MD region in the center of the MD-FEM coupled model. The GB interface in the MD region is visualized as a line of blue and red atoms, indicating atoms in a disordered or hcp surrounding, respectively, reflecting the non-crystalline structure of the GB interface. In Figures 8(a) and 8(b), the crack propagates through the FEM mesh, sequentially opening the CZM elements placed on its path. In Figure 8(c), the crack tip enters the MD domain. The snapshot has captured the instant when the debonding of the surface and interface MD Regions has begun in unison with the opening of the last CZM element on the left side of the MD-FEM interface. The crack tip is about to enter the inner MD region and to continue its propagation in a fully atomistic way. In Figure 8(d), decohesion of the GB in the inner MD region has begun. Shortly afterward, in Figure 8(e), plastic processes start to develop in terms of nucleation of a pair of dislocations, seen as two short blue lines, marking the extended dislocation cores on both sides of the crack tip. Figure 8(f) presents the crack propagated well inside the MD domain. Active dislocation nucleation has already developed and accompanies the crack's propagation. An important result of this process, shown in Figures 8(a-f), is the preservation of the structural continuity between the atomistic and the continuum domains at the MD-FE interface through the entire process of crack propagation from the FEM to the MD systems.

The issues related to coupling the dynamic response of the MD domain to the static response of the FEM system are discussed in detail in Saether, et al.^{17,18} While the dynamic coupling in the ESCM approach cannot be fully achieved without the use of a dynamic FEM simulation, the iterative scheme of coupling, in which the FEM state is continuously updated in accordance with the reported MD displacements, appears to be sufficient to reproduce the evolution of systems with relatively slow dynamics.

Development of Traction-Displacement Relationships from ESCM

In the original purely MD simulation²¹ that was used to obtain CZM relationships, model size restrictions resulted in a finite geometry distortion. The model was limited to a domain of approximately 120 nm x 97 nm x 3 nm and required the application of extremely large applied stresses (approximately 4 GPa) to grow an initial crack that was only a few nanometers in length.

The hydrostatic stress was applied corresponding to fixed displacement boundary conditions before the crack was introduced. Because of the extremely large stresses, hydrostatic loading was required to suppress bulk plasticity.

In contrast, the enhanced ESCM simulation allows uniaxial far-field loading to be applied and eliminates the finite geometry distortion but has only been implemented for the “brittle” crack tip. The procedure for the determination of the CZM parameters of the brittle crack tip using the coupled MD-FEM simulation is the same as that used in the purely MD simulation. The insert in the bottom half of Figure 9 shows a schematic diagram of the discretization of the system volume in the MD simulation into CZVEs for extracting the parameters for the CZM elements. As in Figure 6, Figure 9 shows the $\sigma_{yy}^s(x)$ and $\lambda(x)$ profiles that represent the traction and opening displacement at a single instant of time during crack propagation. The stress profile immediately ahead of the crack tip follows a $1/\sqrt{x}$ type distribution.

A comparison of the recomputed brittle Mode I CZM with the initial pure MD results from Reference 21 is presented in Figure 10. The ESCM-determined traction-displacement curve shows a very large but finite slope until the peak traction of approximately 6 GPa is reached. In contrast, the MD-determined curve begins at approximately 4.25 GPa, corresponding to the value of the hydrostatic pre-stress used in the simulation, and reaches a peak value of approximately 5 GPa. The remainders of both curves consist of a softening region followed by complete unloading (corresponding to the formation of a stress-free surface) at just over 2 nm.

IV. Grain-Scale Idealization

The CZM relationships extracted from the ESCM analysis contain many idealizations (e.g., absence of defects) along the crack plane and cannot be deemed as being quantitative; however, they do improve our understanding of the underlying mechanisms of damage at very small length scales. Additionally, since the selected $\Sigma 99$ GB is believed to be representative of a common class of GBs, additional insight into the mechanisms of intergranular fracture may be gained by implementing the CZMs within a microstructural analysis.

Figure 11a shows a demonstration problem consisting of a 2-D configuration of a tessellated polycrystalline microstructure having many grain boundary interfaces. The model dimensions are $l_x = l_y = 47.5$ nm encompassing 50 grains.²⁶ CZM parameters characterizing the brittle Mode I crack tip behavior of the MD-generated results were extracted from the relationships shown in Figure 10 and (for the purposes of this demonstration) are assumed to apply to all grain boundaries regardless of orientation. These parameters are shown in Table 1, and the constitutive behavior of the resulting idealized CZM is shown by the red curve in Figure 11b.

Table 1. CZM parameters approximating brittle Mode I behavior at the crack tip

CZM	Brittle Mode I
δ_{mx}^o (GPa)	5.00
δ^o (nm)	0.2
δ_{mx}^c (nm)	2.17

Using brittle Mode I CZM properties for all the GBs, Figure 12 shows the sequence of decohesion processes under normal applied displacements with the opening being exaggerated in the figure. An examination of the decohesion processes exhibited in the simulation presented in Figure 12 shows the initial opening of GBs under normal applied displacements. The initial opening of the GBs is shown in Figure 12a. At higher applied strains, the energetics of GB opening dictate the location at which a dominant crack begins to form (Figure 12b). At a critical applied strain, the local coalescence of GB opening forms a dominant microcrack as shown in Figure 12c. After the dominant microcrack has fractured the model, the elastic stiffness in other CZM elements acts to return them to an unloaded state.

V. Summary

New approaches to both concurrent and sequential multiscale modeling have been developed. A new approach to concurrent MD-FEM coupling uses statistical averaging of the atomistic MD domain to provide displacement interface boundary conditions to the surrounding continuum FEM domain, which, in return, generates interface reaction forces applied as piecewise constant traction boundary conditions to the MD domain. Additionally, a new approach to sequential multiscale modeling was developed and based on the definition of a cohesive zone volume element (CZVE). The CZVE is an atomistic analog to the cohesive zone models (CZM) that are often used to model material degradation in continuum finite element analyses. Taken together, these two approaches are an attempt to recast atomistic processes within a format suitable for inclusion in grain-scale finite element analyses and are providing a necessary step toward true physics-based analysis of damage processes.

An application of the ESCM, enhanced by the addition of CZM elements along the crack plane, was presented for analysis of a $\Sigma 99$ GB in aluminum. The model incorporated an edge crack with the tip propagating into the inner MD region of ESCM. The continuity of the crack propagation process through the MD-FEM interface was achieved by the derivation of the CZM constitutive relation for interface debonding using CZVEs and moving averages based on an earlier pure molecular-dynamics simulation. CZM parameters for Mode I fracture were determined and compared with those determined from a pure MD simulation. For a “brittle” crack tip, the peak stress was increased slightly in the ESCM simulation but the overall energy and functional form of the CZM was closely reproduced. Finally, the MD-derived CZMs were used to model intergranular fracture of a highly idealized microstructure.

VI. Acknowledgments

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VII. References

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VIII. Figures

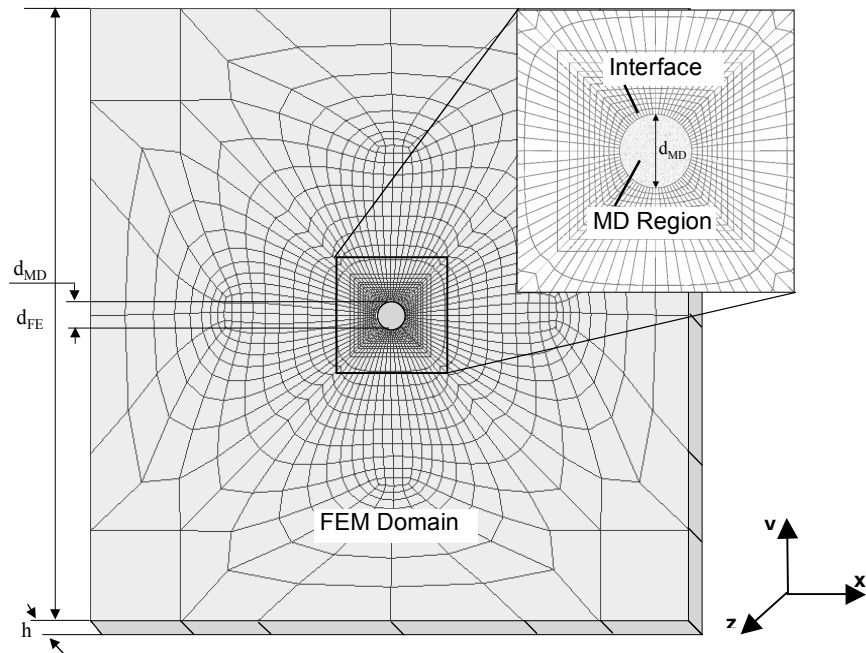


Figure 1. An MD region embedded within a FEM domain

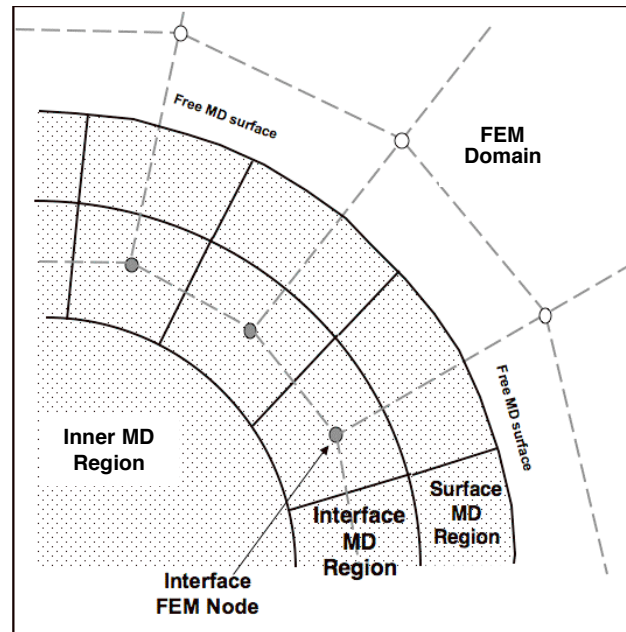


Figure 2. Structure of embedded statistical coupling method

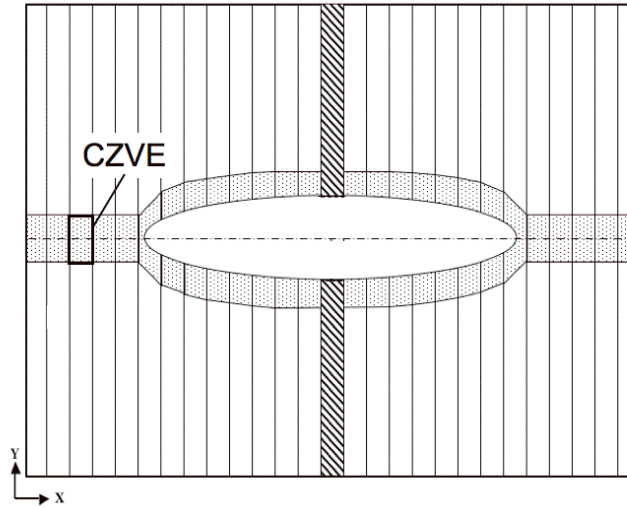


Figure 5. Schematic diagram of the volume slicing and CZVE regions in the MD simulation of a $\Sigma 99$ grain boundary

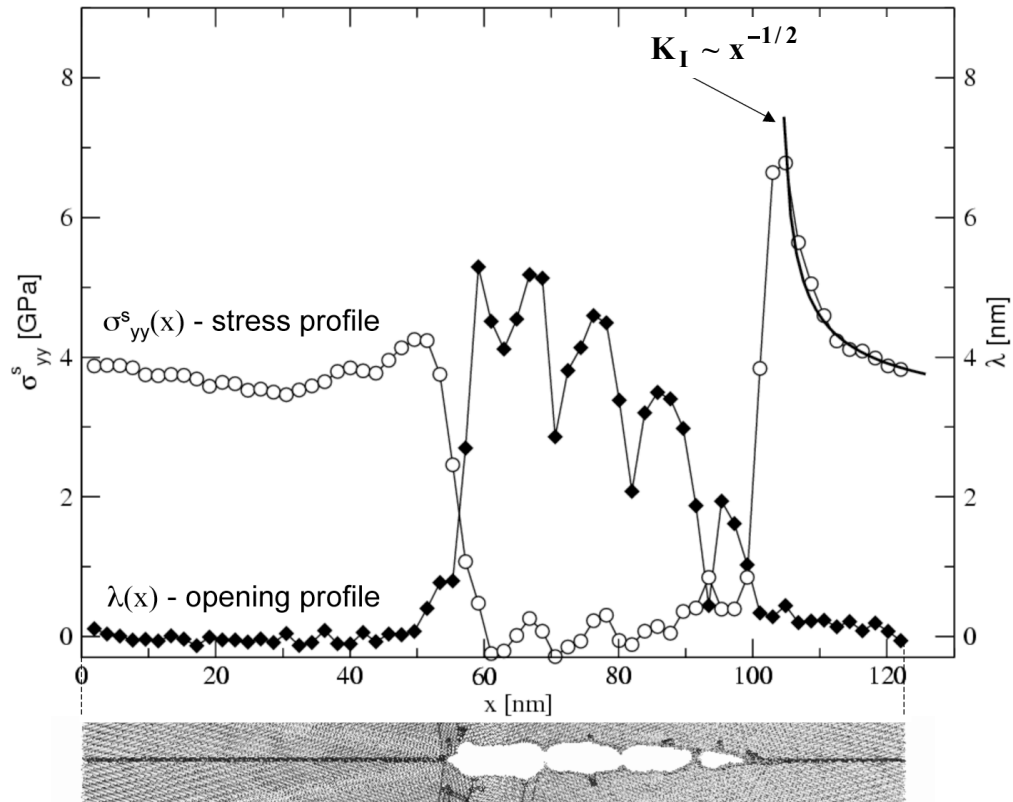


Figure 6. Stress and opening profiles extracted along an embedded crack growing in a MD simulation. A snapshot of the corresponding crack configuration is shown at the bottom of the figure.

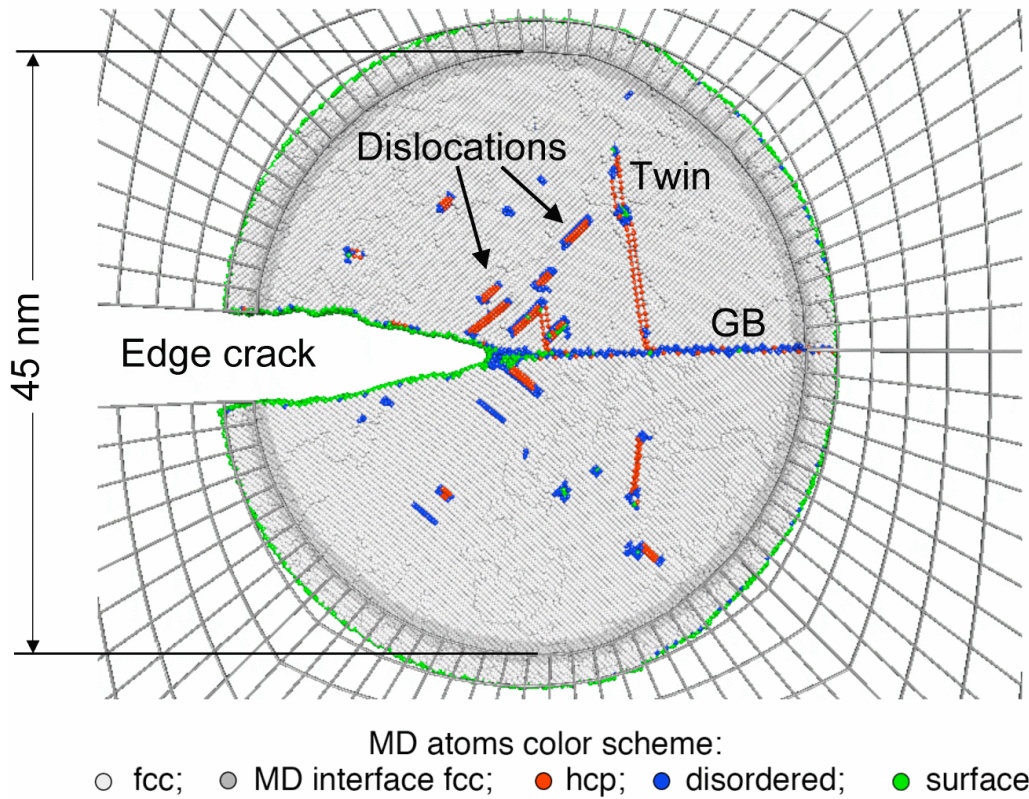


Figure 7. ESCM simulation of an edge crack propagating along a $\langle 110 \rangle$ $\Sigma 99$ symmetric tilt grain boundary in aluminum for 2.0% far-field uniaxial strain

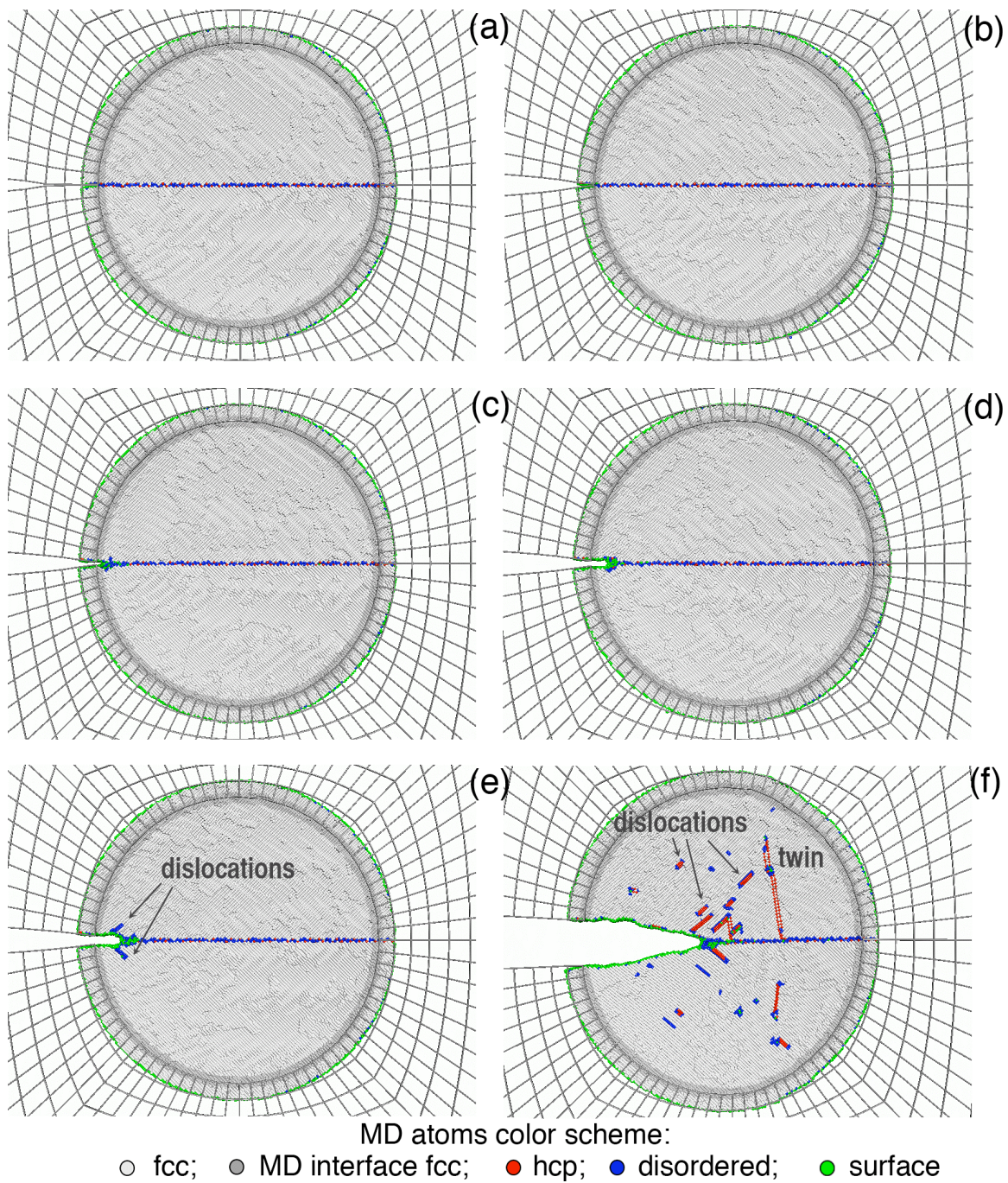


Figure 8. Snapshots of the ESCM model configurations simulating an edge crack propagating along a GB in a bicrystal of aluminum with CZM elements along the GB interface

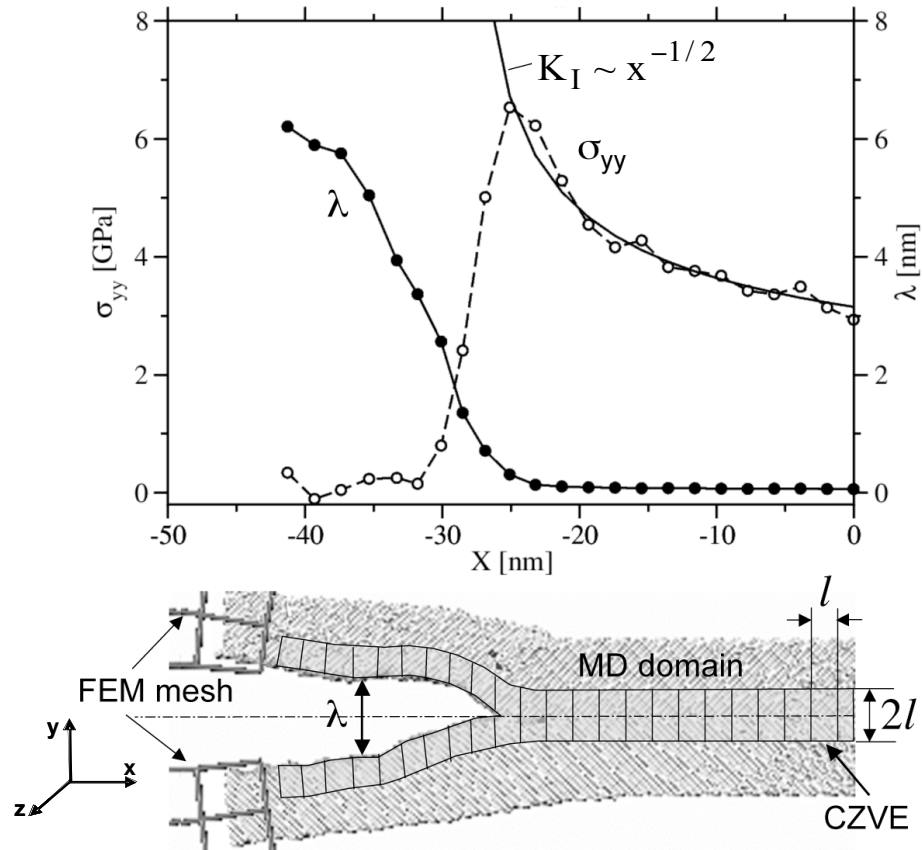


Figure 9. Stress and opening profiles extracted from cohesive-zone-volume-elements (CZVE) placed along the path of an edge crack growing along a grain-boundary inside the molecular dynamics region

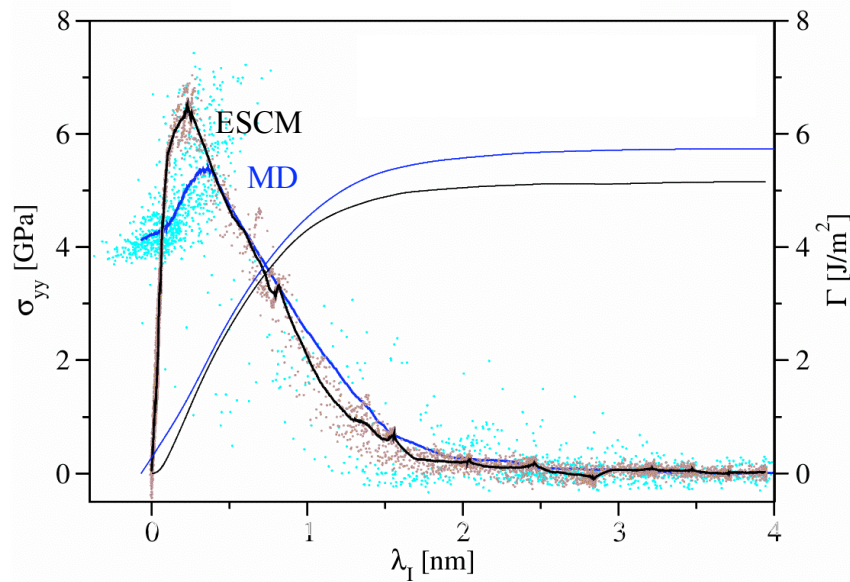
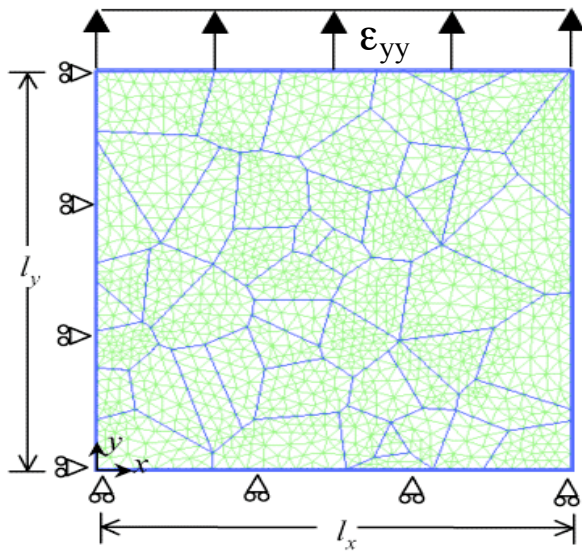
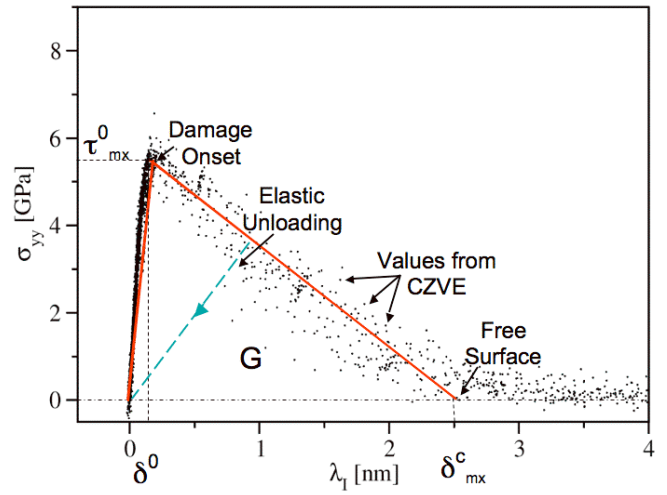


Figure 10. Comparison between the brittle CZM derived using MD and ESCM models

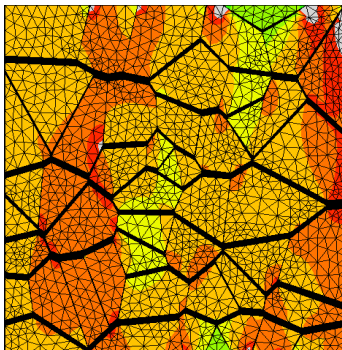


(a) Idealized microstructure

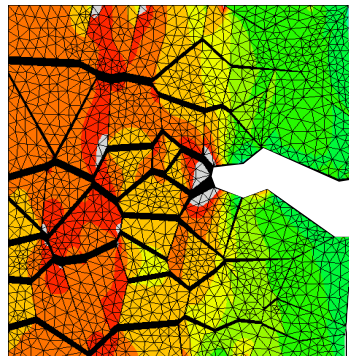


(b) Idealized CZM

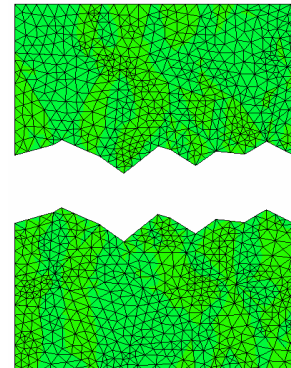
Figure 11. Idealizations of microstructure and cohesive zone model



(a) Initial opening of GBs
 $\epsilon_{yy} = 16\%$



(b) Local crack formation
 $\epsilon_{yy} = 17\%$



(c) Dominant microcrack
 $\epsilon_{yy} = 22\%$

Figure 12. Process of dominant microcrack formation in a polycrystal model simulated using idealized cohesive zone models