

Viewpoint: Challenges to Model the Role of Heterogeneities on the Shock Response and Spall Failure of Metallic Materials at the Mesoscales

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Abstract: The predictive modeling of the experimentally observed behavior of metallic materials under shock loading conditions (wave structures, spall strengths) is a critical challenge towards the design of next-generation structural materials. This challenge is due to the lack of computational methods that can predict microstructural evolution at the mesoscales under dynamic loading conditions. While classical molecular dynamics simulations have been able to provide atomic-scale insights in the defect and damage nucleation/evolution mechanisms, the capability to have a direct comparison with experimental data at the same time and length scales is still a challenge. The current computational approaches require that several approximations be made either for the loading conditions or for the micromechanisms related to defect evolution and interaction at the mesoscales. This viewpoint discusses the insights obtained from molecular dynamics simulations of shock deformation and spall failure of heterogeneous metallic microstructures. An example Al-Ni microstructure is used to identify the critical atomic-scale phenomena that need to be addressed by the mesoscale methods when considering shock deformation and failure (spallation) at the mesoscales.

Keywords: Shock deformation, spall, molecular dynamics, mesoscale

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I. Introduction

One of the long-standing problems in the design of next-generation structural metallic materials is the predictive modeling of defect/damage evolution in extreme environments of high strain rates, high pressures, and shock. Such a capability for predicting the behavior of structural materials will enable the understanding of the response of next-generation blast and penetration resistant materials (BPRMs) under ballistic/blast impact as well as for weapon materials subjected to nuclear weapon operation extremes. These extremes arising from blast/ballistic impact and nuclear shock make it critical to understand the behavior of structural materials at strain rates that are greater than 10^5 s^{-1} . The mechanisms responsible for plastic deformation and failure of structural metallic materials at high strain rates are complex and are affected by heterogeneities in the microstructure that comprises the distribution of grain boundaries, interfaces, and pre-existing densities of defects.

Recent capabilities to synthesize composite metallic materials [1-8] opens opportunities to unravel the role of interfaces distributed in a microstructure with variations in size and structure on the dynamic response. Shock compression behavior of such composite microstructures is observed to be determined by distributions of interfaces that affect defect nucleation/evolution mechanisms and generate mesoscale heterogeneities in the microstructure. The distribution of these mesoscale heterogeneities can provide either strengthening behavior or void nucleation sites and influence spall failure behavior. Tailoring of the response, therefore, requires an understanding of not only the atomic-scale mechanisms of defect nucleation and evolution behavior but also the role of collective distributions of heterogeneities such as porosity, pre-existing defects, interfaces, etc. during shock compression and the role on the void nucleation and growth mechanisms during spall failure. The shock compression response and spall failure of such heterogeneous microstructures is a complex phenomenon that involves modifications in the evolution of defect densities as well as changes in temperatures, phase stability, and wave propagation behavior. While there are several mesoscale models developed in the community based on “continuum-type” descriptions of microstructure [9-11], the applicability of these methods relies on accurate approximations to represent the physics of the processes involved. While such approximations have been successful for the modeling of pure systems [12-16], such approximations become challenging in cases where experimental data on the characterization of deformation mechanisms

is limited. While atomic-scale insights into the defect (dislocations, faults, twins) and damage (voids) evolution behavior are now available using classical molecular dynamics (MD) simulations [17-25], the applicability is limited to single-crystal systems and polycrystalline systems with grain sizes smaller than a hundred nanometers and timescales on the order of tens of picoseconds [26]. For example, the current state-of-art experimental capabilities use *in situ* femtosecond XRD characterization of deformation mechanisms under shock loading conditions [27-29], but this capability only investigates the temporal domains of ~every 150 nanoseconds. The current state-of-art characterization capabilities, therefore, lack the support of mesoscale modeling methods at the relevant length and time scales.

This gap at the mesoscales poses a critical challenge in the development of theories to model microstructural evolution, especially under dynamic loading conditions. The current challenge is in the predictive modeling of alloy microstructures with a distribution of phases with complex deformation mechanisms such as deformation twinning/de-twinning behavior [27, 28] and/or phase transformation [30-33]. This viewpoint discusses the critical atomic-scale insights in the role of heterogeneities such as porosity and interfaces that are important from the point of consideration of mesoscale models to predict dynamic behavior. These insights from MD simulations rely on the availability of computationally efficient interatomic potentials that can accurately reproduce micromechanisms of shock deformation and failure [34-36]. The critical challenges for mesoscale models are outlined below and demonstrated using an exemplar MD simulation of shock deformation and spall failure of a heterogeneous Al/Ni alloy microstructure with a distribution of interfaces and porosity.

II. Dynamic Deformation of Heterogeneous Microstructures at Atomic Scales

Large-scale MD simulations can unravel the role of heterogeneities on the mechanisms related to evolution of dislocations as well as phase transformation behavior that determine the shock response (wave structures, temperatures, and spall strength). A shock is typically generated using a thin piston at one end of the sample that is driven into the sample for a certain duration to mimic loading pressures and/or strain rates of plate impact or laser-shock experiments. Four distinct stages of shock wave propagation behavior are observed in these simulations that are important for validation of mesoscale models:

Shock Compression: The shock compression wave travels through the metal that results in nucleation/evolution of dislocations, faults, twins, etc. behind the shock front. It is now known that loading conditions and initial microstructure determine the evolution and distribution of defects as the shock wave travels through the metal. It is very difficult to model the shock response of heterogeneous microstructures accounting for the decay of the elastic precursor [37-39] as well as twinning [27] and phase transformation [32] in HCP and BCC microstructures.

Shock Release: The end of the shock pulse generates a tail at the piston-end of the metal that follows the compression wave. The compression wave interacts with the rear surface and allows for an expansion of the compressed metal at the back end of the metal. This expansion generates a “reflected” release wave that propagates through the compressed metal towards the piston-end. The critical challenge, therefore, here is the capability to model the propagation of the release waves through the shock modified microstructure that results in annihilation/dissociation/recombination reactions of dislocations, deformation twinning/de-twinning behavior as well as reverse phase transformations in HCP and BCC microstructures [27, 28].

Damage Nucleation: Multiple voids nucleate in the region where the two release waves interact that generate triaxial tensile pressures. Voids nucleation sites in this region referred to as the spall plane and comprise of heterogeneities such as grain boundaries, triple junctions, intersections of defects, stacking fault intersections, twins, as well as interfaces. The critical challenge here, therefore, is to identify and model the contributions of these heterogeneities to void nucleation sites and stresses, that change with microstructure and loading conditions. While experiments are unable to characterize this behavior, the spall strength values are identified as the peak tensile pressures generated and can be used to validate the mechanisms of void nucleation for a given set of loading strain rates, shock pressures, and temperature. [40-43].

Damage Evolution: This stage, also referred to as the *onset of spallation*, corresponds to the formation of void aggregates due to individual voids that grow and coalesce with each other in the spall plane. The current understanding is limited to the post-shock characterization of void sites and size distributions [43, 44]. The critical challenge here is to model the mechanisms of dislocation density evolution and/or twinning/de-twinning behavior during void growth and

coalescence under triaxial tensile pressures that are determined by microstructure and loading conditions.

This section demonstrates the various stages discussed above for an exemplar MD simulation of shock compression and spall failure of a heterogeneous microstructure consisting of a randomly oriented Ni grain embedded in a polycrystalline Al matrix with a pre-existing pore. Figure 1 shows a section of the 50 nm grain-sized system along the sample length, where the atoms are colored based on the total energy of each atom. The system is periodic in the lateral (X and Y) directions and free in Z directions. The lateral dimension is large enough and the system is polycrystalline to eliminate image interactions. The interatomic interactions are defined using the EAM potential for Ni-Al [34] and the simulation is carried out using an in-house MD code. A piston is driven inward at 1 km/s for 10 ps to generate a shock wave with a pressure of ~ 18 GPa. Figure 2 (a) shows the temporal evolution of the structure of the shock front. The end of the shock pulse (10 ps) generates a release wave at the left end of the metal that follows the shock front as it interacts with the pore. The *shock compression* stage shows that the interaction of the shock with the pore results in pore collapse and a change in the shock structure. This interaction results in pore-collapse and increased temperatures, which melt the metal in the vicinity of the pore behind the shock, as shown in Figure 2 (b). Figure 3 shows illustrative snapshots of the system at three points in time during shock compression, where the atom color corresponds to total energy per atom. *Shock release* at the piston-end (tail) occurs after 10 ps and after ~ 20 ps at the rear end of the metal. The release wave interact with each other at ~ 28 ps in the vicinity of the Ni grain. *Damage nucleation* and *damage growth* occur at the Al/Ni interfaces as shown in the snapshots of the system in Figure 4. The temporal evolution of pressures and temperatures along the length of the sample are plotted in Figure 5 and can be used to identify shock pressures (red) and velocities, the wave interaction behavior as indicated by intersecting arrows, the spall strength of the metal i.e. peak tensile (blue) pressures, as well as temperatures generated in the metal during various stages of shock loading and spall failure [22, 25]. The plots show short durations of increased temperatures in a very narrow pore-collapsed region (~ 1000 Å, and ~ 15 -22 ps) followed by rapid drop in temperatures during the propagation of the tail of compression wave. Peak temperatures are also observed in a larger region under triaxial tensile pressures (~ 1000 - 1400 Å, and > 43 ps) due to growth and coalescence of voids.

The mechanisms of pore collapse that render increased temperatures, as well as affect the mechanisms and sites/stresses of void nucleation and related temperature evolution, are therefore, very challenging to predict without running MD simulations and, hence, pose a critical challenge for the development of mesoscale models. The void nucleation sites/stresses cannot be pre-determined as they change with microstructure or loading conditions and remain to be the critical bottleneck in the predictive capability of mesoscale models of dynamic failure of complicated microstructures. In addition, the predictive capability of MD simulations, determined by the interatomic potential, needs validation to gain confidence in the atomic scale insights. The unavailability of such insights for heterogeneous microstructures poses another challenge for models to predict shock deformation and failure behavior at the atomic scales as well as the mesoscales. Significant experimental efforts are required to investigate how multiple types of defects interact, phase stability, and phase evolution [45-52] as well as in-situ characterization of the temporal evolution of microstructure/pressure [27-29, 32, 53-55] under shock loading conditions.

III. Critical Capabilities of Mesoscale Models

The mesoscale models that aim to model dynamic response of heterogeneous microstructures comprising of pre-existing defects, interfaces, pores, etc. need to make approximations for the links between initial microstructure and temporal evolution of defects (dislocation plasticity, deformation twinning, etc.) which result in damage nucleation/evolution and spall failure. Also, of importance, are the capabilities to predict heat generation and transfer that further affects the *shock compression behavior* and *damage nucleation stresses* required for void nucleation as well as the interplay between void growth and coalescence during *damage growth*. In particular, mesoscale models, based on MD insights, must be able to accurately represent the following criteria:

- Reproduce the MD-predicted temporal evolution of atomic-scale characteristics such as the Burgers vectors for dislocations and orientation effects for twinning, for the various dislocations/twins variations for variations in microstructures;

- Reproduce the MD-predicted temporal evolution of relative densities or fractions to incorporate the defect nucleation, interaction, annihilation, recombination, dissociation mechanisms;
- Reproduce the MD-predicted role of microstructural heterogeneities responsible for void nucleation and growth;
- Reproduce the spatial and temporal evolution of temperatures during shock compression of the metal as well as nucleation and evolution of damage as predicted using MD simulations; and
- Reproduce the heat dissipation and transfer, phase transformation behavior, and the spatial and temporal evolution of phases under the wave propagation behavior as predicted using MD simulations;

Mesoscale models with these capabilities will render accurate Hugoniot relationships, shock wave structures, shock rise times, Hugoniot elastic limit values, decay of the elastic precursor, the release and reflected wave velocities wave, spall widths, the evolution of void fractions, and spall strengths for heterogeneous microstructures as predicted using MD simulations.

A newly developed “quasi-coarse-grained dynamics” (QCGD) [56] method uses scaling relationships to coarse-grain atomistic microstructures and reduced number of representative atoms (R-atoms) to expand the capabilities of MD simulations to the mesoscales. The QCGD simulations reproduce MD-predicted temporal evolution of shock structures and the evolution of dislocation density fractions, dislocation reactions and interactions in single crystal and polycrystalline Al [57-59] and Ti [60] microstructures at a significantly lower computational cost. Future work will aim to demonstrate QCGD scaling relationships to model multi-component interactions and predict the mechanisms of pore collapse and role of interfaces during shock compression and spall failure of heterogeneous microstructures.

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FIGURES AND FIGURE CAPTIONS

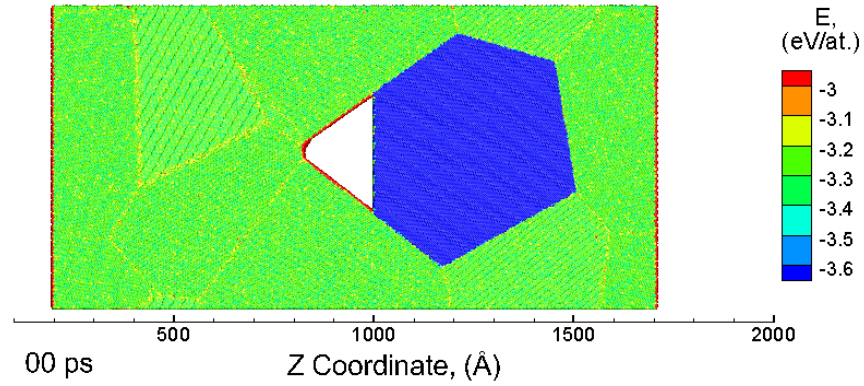


Figure 1: Section from an initial microstructure showing the location of a Ni grain (blue atoms) and an initial void. A piston (left) is driven inward at 1 km/s for 10 ps to generate the shock wave; the atom color corresponds to total energy per atom.

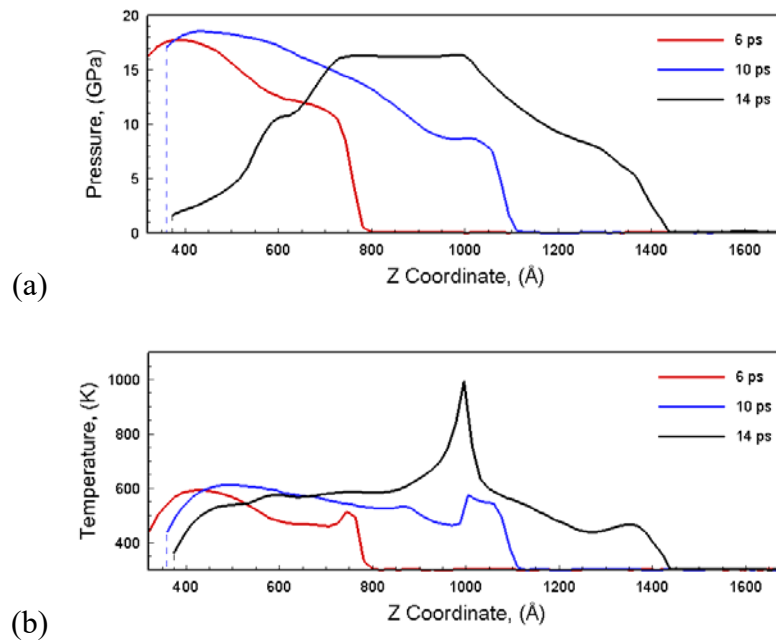


Figure 2: The evolution of pressure and temperature along the sample length under shock loading conditions of 1 km/s and a pulse duration of 10 ps at times when the shock compression wave interacts with the triangular pore in the metal.

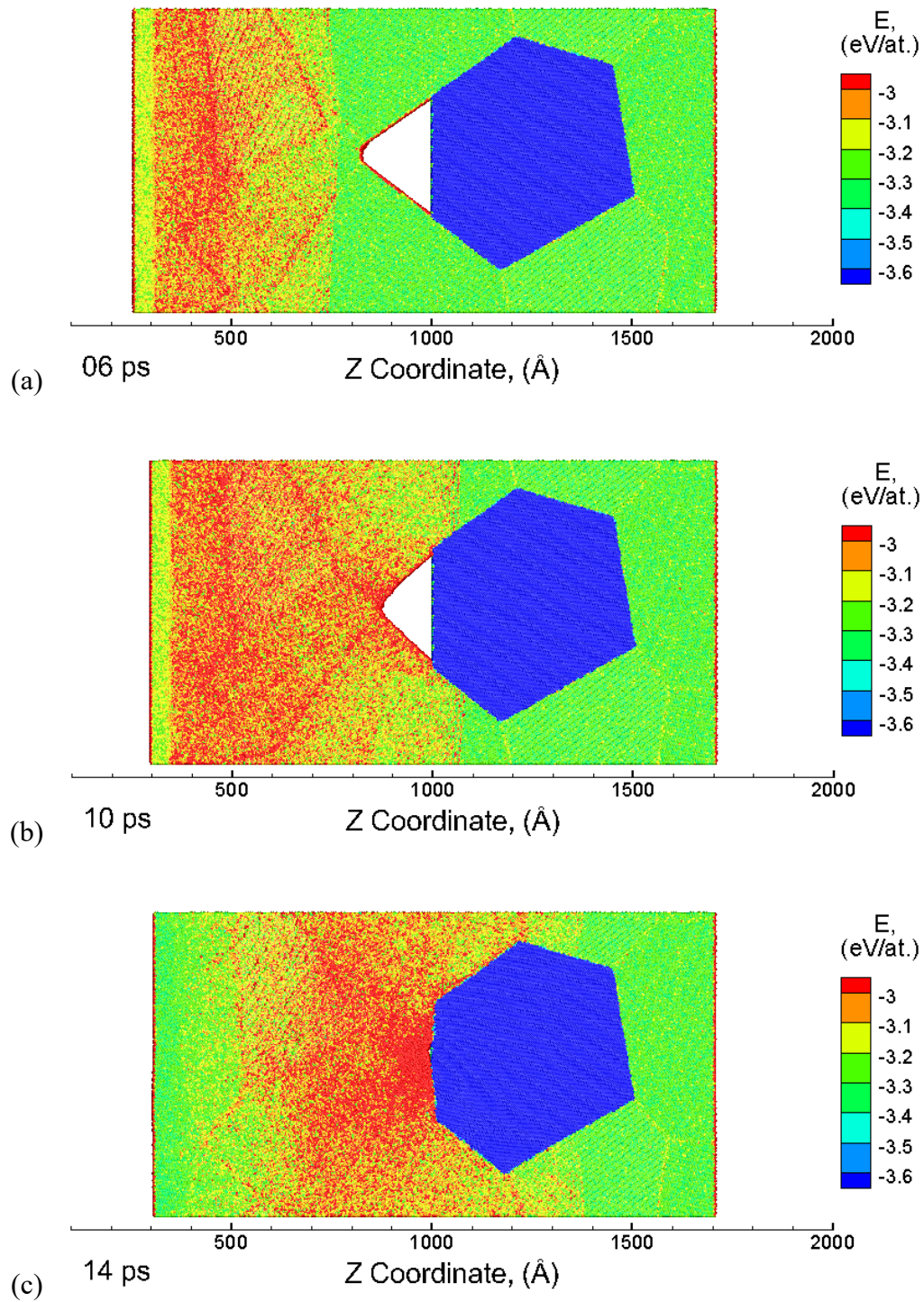


Figure 3: Snapshots showing the interaction of the shock compression wave with a triangular void at times of (a) 6 ps, (b) 10 ps, and (c) 14 ps. The color of atoms corresponds to total energy per atom values.

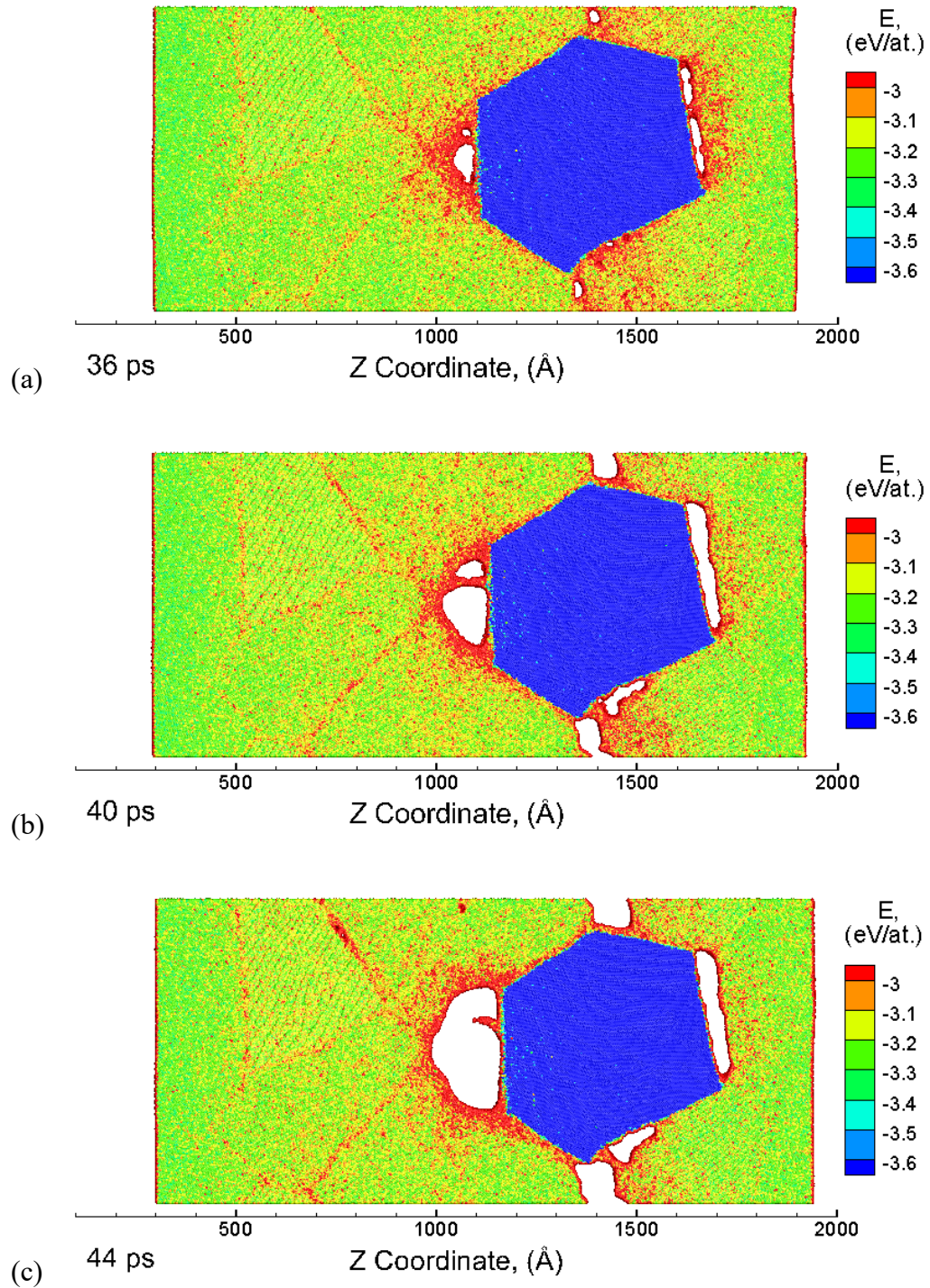


Figure 4: Snapshots showing the interaction of the triaxial tensile wave-wave with an embedded Ni grain that results in nucleation of voids at the Al/Ni interface at times of (a) 36 ps, (b) 40 ps, and (c) 44 ps. The color of atoms corresponds to total energy per atom values.

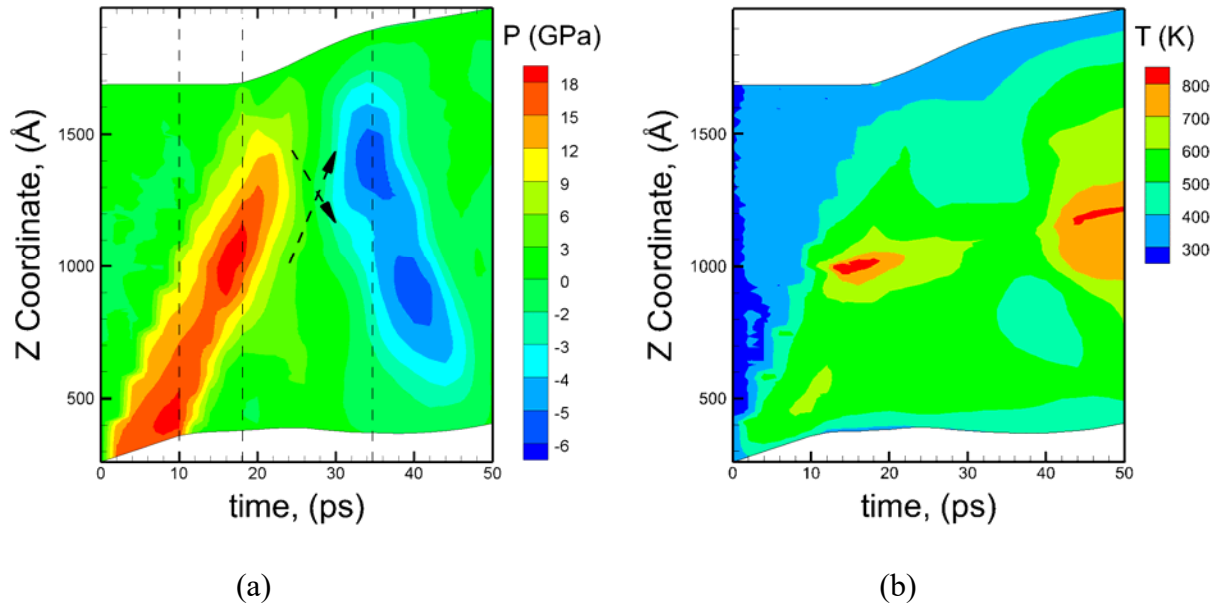


Figure 5: Temporal evolution of (a) Pressure and (b) temperature along the length of the sample in the nanocrystalline Ni/Al system for an impact velocity of 1 km/s and a pulse duration of 10 ps.

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