AMERICAN UNIVERSITY OF BEIRUT

DEFORMATION MECHANISMS IN ALUMINUM SINGLE CRYSTAL: MULTI-SCALE DISLOCATION DYNAMICS ANALYSES

by
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A thesis
submitted in partial fulfillment of the requirements
for the degree of Master of Engineering
to the Department of Mechanical Engineering
of the Faculty of Engineering and Architecture
at the American University of Beirut

Beirut, Lebanon
November 2017

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Date of thesis defense: November 24, 2017

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ACKNOWLEDGMENTS

I would like to thank my supervisor, Professor Mu'tasem Shehadeh, for the advice and guidance he provided throughout my time as a graduate student. I was lucky to have an advisor who cared for my work, and who was always there for support at all times. I would like to thank Professors Samir Mustapha and Kamel Abu Ghali for their support, guidance and inspiring suggestions and recommendations.

I would like to express thanks to my family, who were always there to support me no matter how difficult things got. They were always prepared to give me moral and comfort me during the long nights of work and research. Completing this work would not have been possible without the support of my peers and friends. Finally, I would like to thank the American University of Beirut for all the support.

AN ABSTRACT OF THE THESIS OF

Abdo Mohamad Hamieh for Master of Engineering
Major: Mechanical Engineering

Title: Deformation mechanisms in Aluminum single crystal: multi-scale dislocation dynamics analyses.

Multiscale Dislocation Dynamics Plasticity (MDDP) simulations are carried out to investigate the mechanical response of Aluminum single crystals subjected to extreme conditions. The effects of temperature and strain rate on the dynamic yield point are studied in details. In doing so, an atomistically informed generalized dislocation mobility law is incorporated in MDDP. Additionally, pressure and temperature dependent elastic properties are employed to better capture the shockwave characteristics at elevated temperatures. The simulation results reveal unusual thermal hardening effect along with strain rate hardening behavior. Based on the simulations' findings, a physically based constitutive equation for the dynamic yield strength is proposed. Moreover, we have conducted detailed analyses of the dislocation microstructural evolution and a dislocation density evolution model is presented.

Keywords: dislocation dynamics, shockwave, high strain rate, nucleation, multiscale simulation

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Chapter I
Introduction, Literature and Research objectives

A. Rationale

The behavior of different materials structures under shock waves or high strain rate and as a function of temperature are studied extensively both experimentally and through different simulation methodologies mainly molecular dynamics. Experimental and simulation works are highly interested in understanding the microstructure behavior and the dislocation mechanisms behind the results experiments and simulations are showing.

Ashitkov, Chapman, Garkushin, Kanel, Razorenov, Zaretsky et al. studies experimentally and via simulations the behavior of different metals under temperature and strain rate variations. Thin Iron films under shock loading driven by a femtosecond laser are studied experimentally and by molecular dynamic simulations (Ashitkov, Zhakhovsky et al. 2017). Aluminum alloy AMg6M and pure aluminum samples are loaded by planar shock waves while the test temperature is varied from 20 to 600°C (Razorenov, Kanel et al. 2003). Effect of temperature on the yield stress of different metals under shock compression is investigated (Kanel', Fortov et al. 2007). Single crystal, polycrystalline metals, alloys and their dynamic yield stress growth are studied (Kanel, Razorenov et al. 2004). Copper samples are shock-loaded over 300 to 1353K and the evolution of elastic-plastic shock waves as a function of the propagation distance is considered (Zaretsky and Kanel 2013). Experimental data on elastic precursor decay and rise times in several metals and alloys at normal and elevated temperatures are discussed (Kanel 2012). Unexpected features in the wave evolution in solids and changes of shape of elastic precursor wave as a result of variations in the material

structure and the temperature are discussed (Kanel, Savinykh et al. 2016). Effects of time and strain on material strength are extracted from precise measurement of the free-surface velocity (Chapman, Eakins et al. 2014). Influence of impurities on spall strength is presented (Garkushin, Kanel et al. 2016). HEL rise for Aluminum and copper single crystals over a wide range of strain rates and temperatures is discussed (Razorenov, Kanel et al. 2002). An experimental technique that reveals the different modes of materials behavior under shock wave is presented (Zaretsky, Paris et al. 2003). With initial temperature from 296 to 932K, the evolution of elastic-plastic shock waves with propagation distance has been studied (Zaretsky and Kanel 2012). Experimental results of the dynamic yield strength and dynamic tensile strength of aluminum single crystals shock loaded as a function of temperature are presented (Kanel, Razorenov et al. 2001). With the initial temperature varied from 20 to 648°C, measurements of dynamic tensile strength of aluminum single crystals under shock loading are presented (Kanel, Baumung et al. 2000). The dynamics of the motion of the free surface of micron and submicron films has been investigated (Ashitkov, Agranat et al. 2010). HEL and spall strength of aluminum, magnesium, and zinc over a wide temperature range are analyzed (Kanel, Razorenov et al. 2002). Results of measurements of the dynamic yield stress and the ultimate strength of aluminum single crystals in the temperature range from 15 to 650°C, 10°C lower that the melting point, are presented (Kanel and Razorenov 2001). The shock wave phenomena generated in aluminum films with thickness ranging from 0.5 to 1.2μm is studied, and femtosecond laser pulses are used to induce the shock waves (Ashitkov, Agranat et al. 2012).

Experimental investigations are always more interesting than simulations since their results will be more realistic and meaningful. However, for such high strain rates, experiments are

critical and costing. Still, lots of works in addition to Kanel et al. explore experimentally the field. Remington et al. use high-power pulsed lasers and shocks at pressures of hundreds of GPa up to several TPa and strain rates of $10^6 - 10^{10}\mathrm{s}^{-1}$ (Remington, Remington et al. 2017). Choudhuri et al. examine anisotropy effects at high stresses by shock compressing Al along different orientations (Choudhuri and Gupta 2011). Chen et al. conduct a series of plate impact spall experiments for seven microstructural conditions of aluminum (Chen, Asay et al. 2006). High purity aluminum samples are impacted with a velocity varying from 196.9 m/s to 317.9 m/s by Lan et al. (Mei-Lan, Hong-Liang et al. 2007) and the damage behavior of the samples is analyzed based on the vibrating features of the free surface velocity profiles. The failure of ultrapure aluminum due to nucleation, growth and coalescence of microscopic voids under shock wave loading is studied (Qi, Luo et al. 2012). Plastic flow in Al and Fe thin foils ramp compressed through laser ramp compression are studied and strain rate is varied between$10^6 - 10^8\mathrm{s}^{-1}$ (Smith, Eggert et al. 2011).

Another commonly used approach is molecular dynamics simulations. The melting of Aluminum is studied by Gubin (Gubin, Maklashova et al. 2015). Yanilkin et al. investigate the mechanisms and kinetics of plastic deformation of Al and Al-Cu alloys under strain rates greater than$10^5\mathrm{s}^{-1}$ (Yanilkin, Krasnikov et al. 2014). Krasnikov et al. propose a two level approach for describing the plastic deformation under high rate loading, and in addition to the molecular dynamics simulation at the atomistic level, a model of continuum mechanics is used to describe dislocations and the macroscopic motion of a material (Krasnikov, Kuksin et al. 2010). Kuskin et al. analyze microscopic mechanisms and kinetics of dynamic fracture of crystalline materials based on MD modeling and present the results as kinetic constitutive relations (Kuksin, Norman et al. 2010). Deformation behavior of metallic alloy crystal

nanowires of pure Cu, NiCu, and NiAu alloy under high rates ranging from$5 \times 10^{8}\mathrm{s}^{-1}$ to $5 \times 10^{10}\mathrm{s}^{-1}$ is studied (Qi, Ikeda et al. 1998).

One main driving force for lots of works is to obtain values for parameters to build constitutive equations of numerical simulation models (Kanel, Fortov et al. 2004). In addition to previously mentioned works aiming this target, Loyd et al. extended an existing high strain rate viscoplastic model that tracks the nucleation, multiplication, annihilation and trapping of dislocations (Lloyd, Clayton et al. 2014). Mayer formulated a continuum model of tensile fracture of solid metals for pure aluminum and D16 alloy (Mayer 2016). Krasnikov et al. proposed a continuum dislocation based model of nanovoids growth (Krasnikov and Mayer 2015).

Further, Tang et al. conducted dislocation dynamics DD simulations for Fe at several high strain rates and temperatures (Tang and Marian 2014). Armstrong et al. described the high strain rate dependence of the flow stress of metals from a dislocation mechanics viewpoint (Armstrong and Walley 2008).

Gurrutxaga-Lerma has different works around dislocations and their mechanisms under extreme conditions of temperature and strain rate. He criticized current methods of modeling plasticity as the collective motion of discrete dislocations since they ignore the time dependent nature of the elastic fields of dislocations (Gurrutxaga-Lerma, Balint et al. 2013). A full explanation of what has been known for more than six decades as “the decay of the elastic precursor” is provided (Gurrutxaga-Lerma, Balint et al. 2015). A two-dimensional method of discrete dislocation dynamics aimed at the study of plastic relaxation processes subjected to weak shock loading is presented (Gurrutxaga-Lerma, Balint et al. 2014). The

time to activate Frank-Read sources in response to strain rates ranging from $10^1$to $10^{10}s^{-1}$in aluminum under athermal conditions is examined (Gurrutxaga-Lerma, Balint et al. 2015). The implementation of homogeneous nucleation in dynamic discrete dislocation plasticity D3P is described (Gurrutxaga-Lerma, Balint et al. 2015) since it is the dominant dislocation generation mechanism at strain rates above 10^8s^{-1}. Also, the role of the choice of a dislocation mobility law in the study of plastic relaxation at shock fronts is examined (Gurrutxaga-Lerma 2016).

Shehadeh et al. investigates on different metals. They study the deformation process in copper and aluminum single crystals using a multiscale model of plasticity that couples discrete dislocation dynamics and finite element analyses. Strain rates ranges from $10^5$to 10^7 s^{-1} (Shehadeh*, Zbib et al. 2005). They investigate the deformation process in FCC single crystals under high strain rate ranging between10^5to10^8 s^{-1}. In the first part, the effects of peak pressure are investigated, the shock pulse duration, the crystal anisotropy and the nonlinear elastic properties on the interaction between shock waves and preexisting dislocation sources. In the second part, they focus on shock-induced dislocation nucleation (Shehadeh 2006). Ultra short pulse shock wave propagation, plastic deformation and evolution of dislocations in copper single crystals are investigated for different orientation (Shehadeh, Zbib et al. 2005). Shehadeh and Zbib couple computer simulation with theoretical modeling and available experimental data to determine the underlying physics behind shock induced plasticity. Simulations are run for copper at ultra-high strain rates (Shehadeh and Zbib 2016).

Kattoura (Kattoura and Shehadeh 2014) carries out multiscale dislocation dynamics calculations to simulate the mechanical response of copper single crystals under shock

loading with strain rates ranging from $10^6$to 10^{10} s^{-1}. He considers plasticity mechanisms associated with activation of pre-existing dislocation sources and homogeneous nucleation of glide loops.

B. Background

A process that depends on time is said to be dynamic. Since all processes depend in reality on time, Zukas in his book “Introduction to Hydrocodes” found it very intuitive to say “all processes in life are dynamic” (Zukas 2004). One of those processes and might be indeed of those most interesting, general, and sophisticated in life is the behavior of materials under very high strain rates. It is general because we found it everywhere because materials are everywhere around us. It is interesting simply because it might touch our lives and frequently. It is sophisticated and really sophisticated for many reasons. One is that we have to go to the microstructure of the material to be able to understand it, and we all know that once we go to that level things become more complicated. Another reason is that at this level many parameters can contribute to the material behavior like temperature, load duration, and strain rate.

Meyers in the first chapter of the “Dynamic Behavior of Materials” and through the nice example of the sand bag used to stop bullets in old war movies and its different reactions to both a simple knife, which is a slowly changing load, and a bullet, which is a high speed changing load, illustrates the effect of one of these parameters, which is the strain rate, in a very intuitive example (Meyers 1994).

However, theories cannot be built on such intuitive examples simply because not all examples are so simple. We need to build models based on which experiments and simulations can be easily understood.

C. Shock Waves

Waves are propagation of energy **(**Figure 2**,** Figure 1**,** Figure 3**)**. Since we are dealing here with mechanical waves and not electromagnetic, the propagation of energy will take the form of a propagation of stress through a body. This wave propagation will often involves dynamic deformation of this material. When the material deforms elastically, we talk about elastic waves. When it deforms plastically, i.e. the amplitude of those waves exceeds the elastic limit of the material, we talk about plastic waves (Meyers 1994).

If we refer to Zukas in "Introduction to Hydrocodes", we can define a high-pressure shock wave as a wave that moves at a very high velocity, around 8 km/s, or at velocities exceeding the speed of sound in a material which is usually 6 km/s in metals (Zukas 2004).

If we refer back to the simple "sand bag" example of Meyers, we could intuitively recall that the sand bag defeats the bullet which is moving at a much higher velocity than a knife that can easily penetrate it (Meyers 1994). If we follow philosophers in their way in generalizing the rules of nature, we can compare this material behavior, which is a sand bag here, to the effect of hard work or controlled work stress in making us stronger. However, scientists make the opposite, instead of being satisfied with general rules, which are easy and simple; they need to go deeper inside the material to understand what is happening at the micro level. This is where dislocations show up to help them.

D. What is an Equation of State?

A shock physicist will define it as an attempt to build a relation of mathematical functional form between the theoretical microstructure atomic models and the experimental results and observations of the macroscopic behavior of materials. Zukas in “Introduction to Hydrocodes” published in 2004 claims that no general theory allows going from atomic considerations to prediction of continuum behavior and that is why we introduce simplifications.

As for an engineer, an equation of state would be whatever information about the material that allows proceeding with whatever problem we are trying to solve. This difference between an engineer and a scientist is the difference between engineering and science because engineering is always seeking to come up with plausible answers to impossible problems in a finite amount of time and inadequate budget as Zukas said. (Zukas 2004)

E. Rankine – Huguenot Jump Conditions

Many equations are involved in shock problems to be able to solve it. These are the three conservation equations, conservation of mass, conservation of momentum, and conservation of energy. They contain a total of 8 parameters. Also, they will be added to two more relationships one of which is the previously discussed Equation of State (EOS). The problem will be complete after the specification of boundary conditions. So, mass, momentum, and energy are conserved across the shock front according to the following equations.

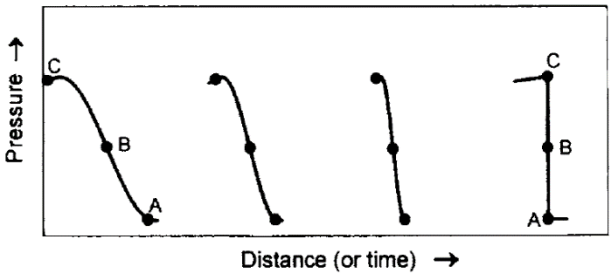


Figure 2: Buildup of a pressure wave to a shock wave (Zukas 2004)

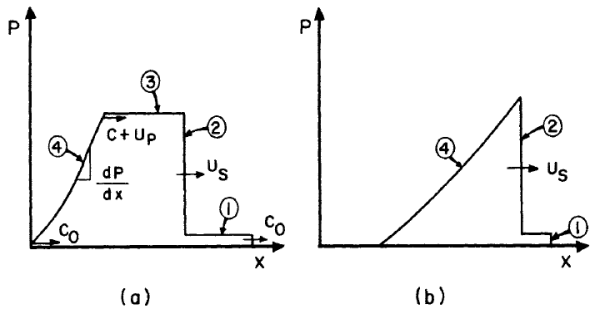
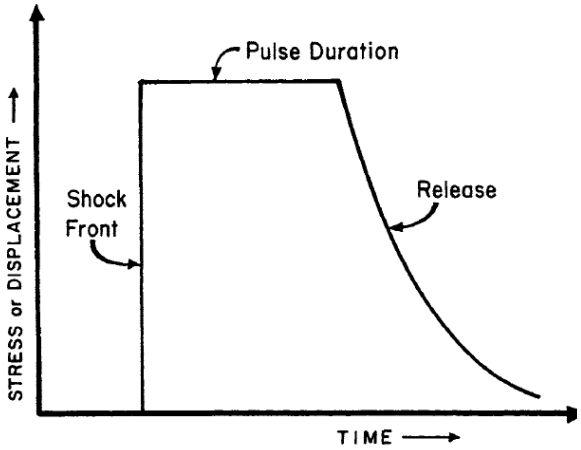


Figure 1: Shock wave configurations: (a) shock wave (trapezoidal) produced by plate impact; (b) shock wave (triangular) produced by explosive detonation or pulsed laser (Meyers 1994)



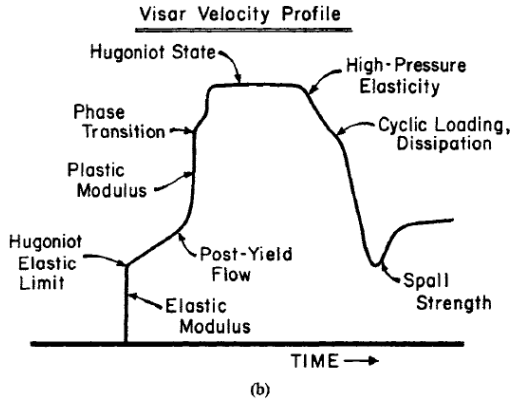


Figure 3: (a) Idealized and (b) "generic" realistic shock wave profile (Meyers 1994)

Table 1: Important Physical Properties of Aluminum

Property	Value
Elastic Modulus	70 GPa
Poisson Ratio	0.33
Shear Modulus	27 GPa
Density	2713.5 kg/m^3

F. Dislocation Theory

Plastic deformation in crystals occurs due to the generation and transport of dislocations (Shehadeh 2006). However, since dislocations are class of defects in crystalline solids, one needs to understand first what crystallinity is (Hull and Bacon 2011). Briefly, and referring to the book of Hull and Bacon, metals and non-metallic solids are said to be crystalline when the constituent atoms are arranged in a simple regular pattern that is repeated periodically in three dimensions (Figure 6). The most common types of crystal structures are the body-centered cubic, face-centered cubic and close-packed hexagonal.

Defects in crystals, or imperfections, which can be point (Figure 4), line, surface or volume defects, will disturb the crystal arrangement and will modify the properties of the material. Our main interest in this study is on dislocations which are line defects, and where first discovered by Orowan, Polanyi, and Taylor in 1934 through the difference between the predictions of theoretical shear strength and its experimental values.

A dislocation line is defined by its Burgers vector (b), which is the displacement of the atoms that occurs in the crystal as the dislocation moves, and line sense, which is a unit vector

tangent to the dislocation line. In an edge dislocation the burger vector will be normal to the line sense, and it will be parallel to it in a screw dislocation (Figure 5, Figure 7).

Dislocations will move on slip planes and slip directions. Slip planes are planes with the highest density of atoms, i.e. those which are most widely spaced. Direction of slip is the one of the shortest lattice translation vectors (Figure 8).

Simulations were done on Aluminum crystals which are face-centered cubic cell structure (FCC) crystals. In FCC crystals, atoms are situated at the corners of the unit cell and at the centers of all cube faces in sites of the type $0, \frac{1}{2}, \frac{1}{2}$ and they touch along the <011> close-packed directions. In crystals, cell dimensions are the lattice parameters, which define with the different angles the size and shape of the cell. So, in an FCC crystal, the lattice parameter isa $= 4\mathrm{r}/\sqrt{2}$.

One topic in Dislocation theory, which is of interest in our study, is the multiplication and generation of dislocations. This can take place through different mechanisms one of which is the “Frank – Read sources”. Physically, the regenerative multiplication of dislocations takes place to account for the large plastic strain produced in crystals (Hull and Bacon 2011) (Figure 11, Figure 12).

Cai in “Dislocation Core Effects on Mobility” (Cai, Bulatov et al. 2004) discussed in a chapter the atomic structure and interactions in the dislocation core and their effects on dislocation mobility. He defines the Peierls stress as the minimum stress required for the dislocation to move. Consequently, it will be related to the macroscopic yield stress above which the crystal starts to deform plastically. However, Peierls stress does not take into account temperature effect but is more an idealized concept at zero temperature while in

reality and according to basic physical laws, the motion of a dislocation is a function of temperature and the time of the motion. Another measure of lattice resistance to dislocation motion is the Peierls barrier or Peierls valley defined as the energy barrier that a straight dislocation must surm+ount to move to a neighboring lattice. Much of FCC metals and alloys dislocation behavior is due to Shockley dissociation, the split of a dislocation into two partial dislocations surrounding an area of stacking fault **SF,** and is expressed in Miller index notation as:

$$\frac{1}{2}[110] = \frac{1}{6}[21\bar{1}] + \mathrm{SF} + \frac{1}{6}[121] \ (1)$$

This dissociation results in a considerable reduction of elastic energy. According to Hull and Beacon, a stacking fault is a planar defect and, as its name implies, it is a local region in the crystal where the regular stacking sequence is interrupted.

a. Macro scale continuum mechanics equations

Dynamics and kinetics of dislocation are introduced into continuum mechanics equations which look for 1-D Lagrangian coordinates as follows: (Yanilkin, Krasnikov et al. 2014)

$$\frac{1}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\frac{\partial \mathrm{u}}{\partial \mathrm{z}} \ (2)$$

$$\rho\frac{\mathrm{du}}{\mathrm{dt}} = \frac{\partial \sigma_{\mathrm{zz}}}{\partial \mathrm{z}} \ (3)$$

$$\rho\frac{\mathrm{dE}}{\mathrm{dt}} = -\frac{\sigma_{\mathrm{zz}}}{\rho}\frac{\mathrm{d}\rho}{\mathrm{dt}} + \frac{\partial}{\partial \mathrm{z}}\left(\mathrm{K}\frac{\partial \mathrm{T}}{\partial \mathrm{z}}\right) (4)$$

$$\sigma_{\mathrm{zz}} = -\mathrm{P}(\rho, \mathrm{E}) + \mathrm{S}_{\mathrm{zz}} \ (5)$$

$$\frac{dS_{zz}}{dt} = \frac{4G}{3}\frac{\partial u}{\partial z} - 2G\frac{dw_{zz}}{dt} \quad (6)$$

$$\frac{dS_{xx}}{dt} = -\frac{2G}{3}\frac{\partial u}{\partial z} - 2G\frac{dw_{xx}}{dt} \quad (7)$$

$$\frac{dS_{yy}}{dt} = -\frac{2G}{3}\frac{\partial u}{\partial z} - 2G\frac{dw_{yy}}{dt} \quad (8)$$

$$\frac{dS_{ik}}{dt} = -G\left(\frac{dw_{ik}}{dt} + \frac{dw_{ki}}{dt}\right) \text{at } i \neq k \quad (9)$$

ρ Is the substance density, uis the substance velocity, $\sigma_{zz}$is the full stress decomposed into the pressure P, and the deviatoric partS_{zz}. E and Tare the specific internal energy and the thermodynamic temperature, respectively. K is the heat-conduction coefficient.

b. Dislocation mechanisms of motion and deformation and nucleation

For most metals, under moderate strain rate loadings, the yield point decreases with increasing temperature. The reason is that with the increase of temperature, and through thermal activation, dislocations will be easily able to overcome Peierls barrier that hinders their motion, and thus glide easily. Consequently, plastic flow becomes increasingly easy and yield point drops (Gurrutxaga-Lerma, Shehadeh et al. 2017).

However, all this does not apply for shock loading. First, the magnitude of the applied loads induced by the shock will exceed the Peierls barrier and the ideal strength of the material. Second, the dominant factor during the shocking mechanism, which will activate dislocation motion, will not be temperature but strain rate. As a result, to be able to move, dislocations will not need to overcome Peierls barrier but only lattice resistance that acts on dislocations as a drag force. We say in this case that dislocation motion is dominated by dislocation drag

not thermal activation or the need to overcome Peierls barrier. The so called drag force, dislocation drag, or lattice resistance, is caused by phonon scattering, dislocation radiation, and phonon wind effects. This resistance is proportional to temperature i.e. when temperature increases, the drag increases and dislocation motion is hindered. This is the reason behind the increase of plastic yielding with the increase of temperature (Gurrutxaga-Lerma, Shehadeh et al. 2017).

On the other hand, with the advance of the shock wave it interacts with existing dislocations sources leading to their activation when the shear stress exceeds the critical value to overcome the lattice friction and the self-stress of the activated sources (Gurrutxaga-Lerma, Shehadeh et al. 2017). This leads to the emission of loops and segments from the FR sources with an accelerated velocity reaching instantaneously the shear wave velocity. The source activation takes place uniformly due to the isotropy in the Peierls barrier exhibited by Al, so that all parts of the source begin to bow out at the same time regardless of their character. Consequently, more sources are activated with the wave propagation and more dislocations are emitted from the previously activated sources all this leading to a large increase in the dislocation density at a very high rate relaxing the shock front.

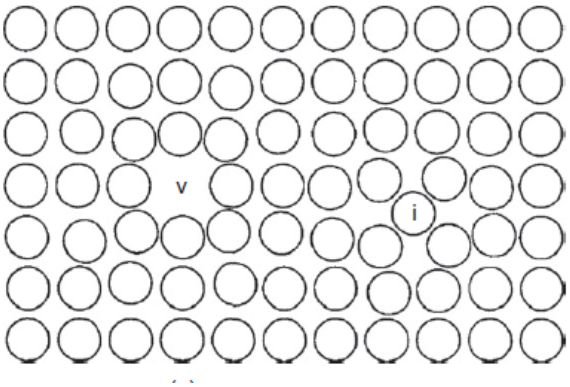


Figure 4: Point defects (Hull and Bacon 2011)

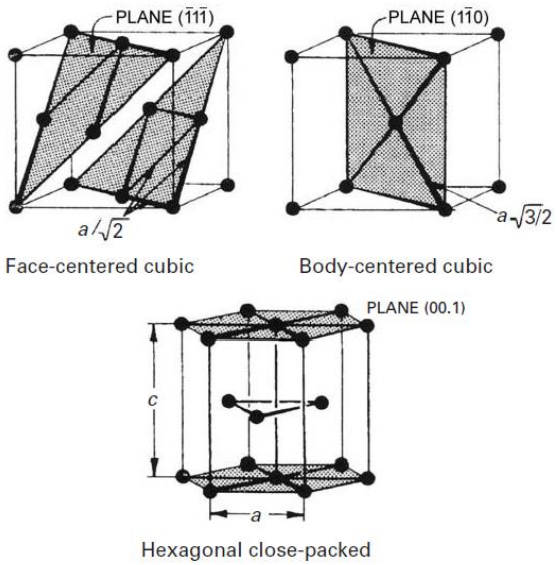


Figure 5: Most closely packed planes in (a) FCC; (b) BCC; (c) HCP (André Meyers 2009)

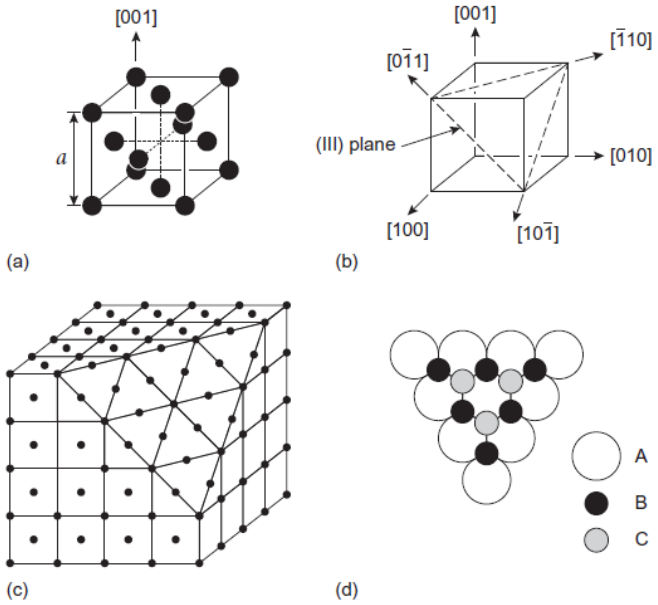


Figure 6: Face-centered cubic structure: (a) unit cell, (b) principal directions, (c) arrangement of atoms in a (111) close-packed plane, (d) stacking sequence of (111) planes (Hull and Bacon 2011)

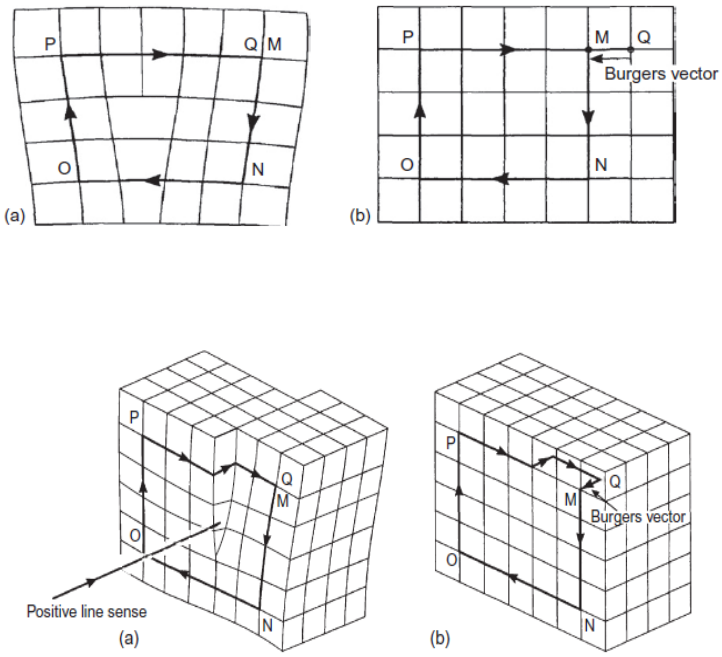


Figure 7: Burgers circuit round an edge (above) and a screw (below) dislocation (Hull and Bacon 2011)

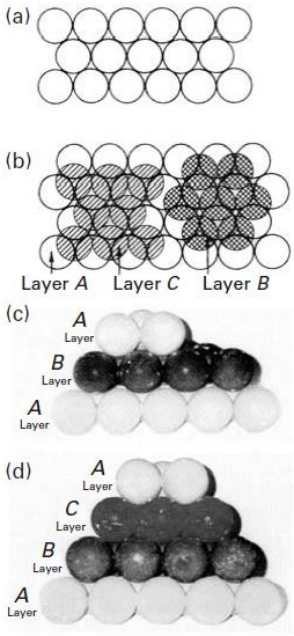


Figure 8: Layers of most closely packed atoms in different crystal structures (André Meyers 2009)

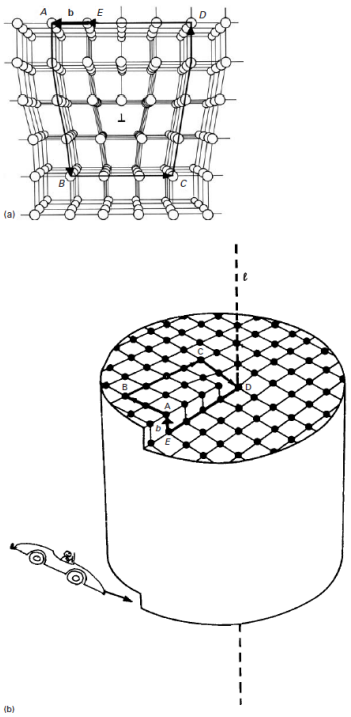


Figure 9: (a) Arrangement of atoms in an edge dislocation and the Burgers vector b that produces closure of circuit ABCDE. (b) Arrangement of atoms in screw dislocation with “parking garage” setup (André Meyers 2009)

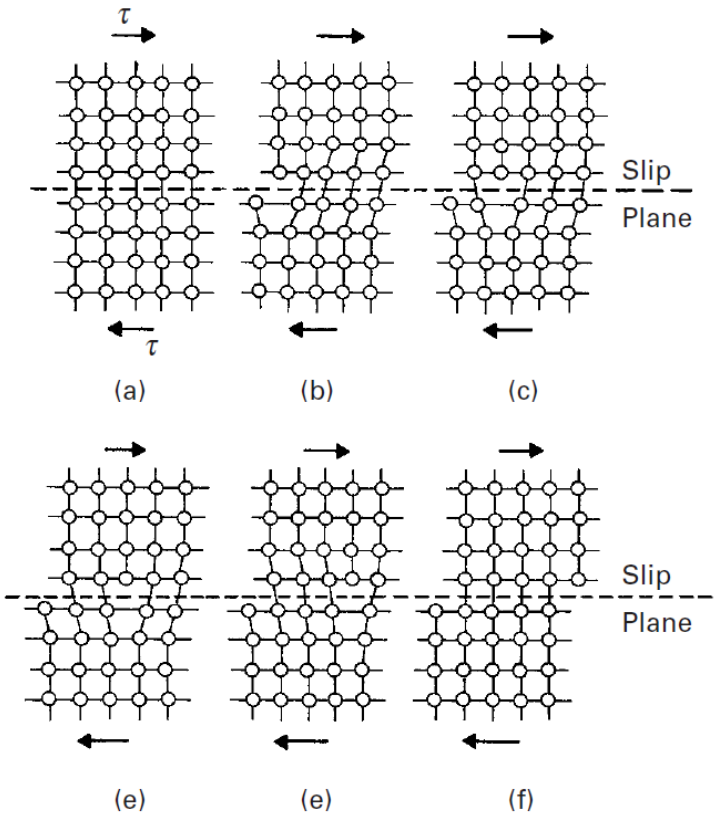


Figure 10: The plastic deformation of a crystal by the movement of a dislocation along a slip plane (André Meyers 2009)

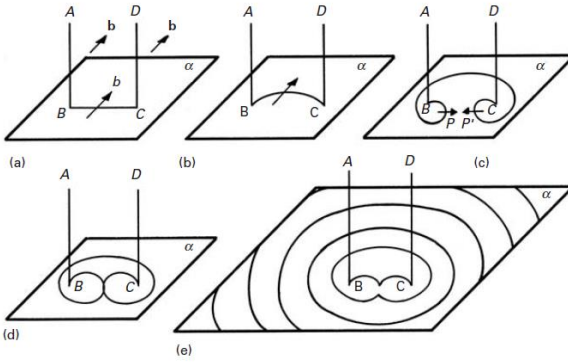


Figure 11: Sequence of the formation of dislocation loop by the Frank-Read mechanism (André Meyers 2009)

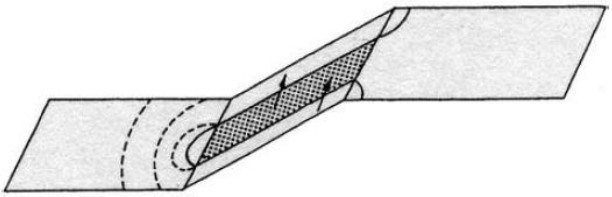


Figure 12: Frank-Read source formed by cross-slip (André Meyers 2009)

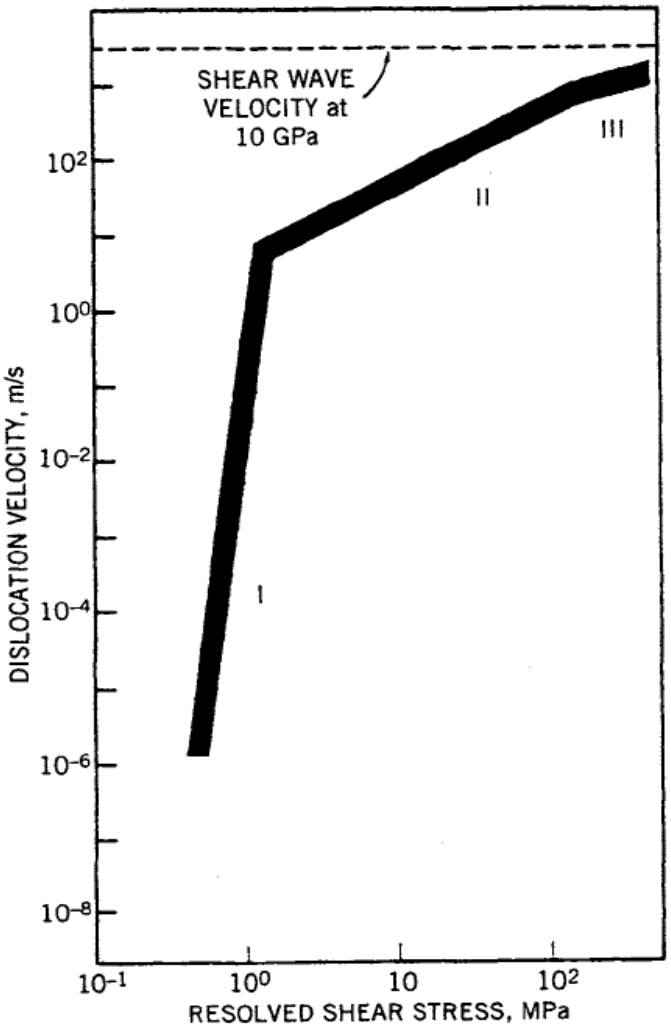


Figure 13: Dislocation mechanisms (Meyers 1994)

Chapter II
Methodology

A. Multi-Scale Dislocation Dynamic Plasticity (MDDP)

MDDP is a model of plasticity that couples discrete dislocation dynamics and finite element analysis. At Washington State University, professor Zbib and collaborators have developed a three-dimensional Dislocation Dynamics codes framework where plastic deformation of single crystals is obtained by the explicit evaluation of dislocation evolution history. Dislocation lines and curves are modeled as discrete straight segments that interact with each other. On each dislocation segment, Peach-Koehler (PK) force resulted from different sources is calculated; forces exerted on the dislocation from externally applied stresses, and the stress fields from neighboring segments and other dislocations in the computational cell.

The mobility of the dislocations is described by a relationship between the segments speed and the applied loads mentioned:

$$f_{PK} = \frac{d(T)}{1 - \frac{v^2}{c_t^2}} v \quad (10)$$

$f_{PK}$is the Peach-Koehler force, vthe glide speed, $d(T)$the drag coefficient, $c_t$the material's transverse speed of sound (Gurrutxaga-Lerma, Shehadeh et al. 2017).

The motion of a dislocation may be encountered by local obstacles: stacking fault tetrahedral, defect clusters, and vacancies. It has to overcome further internal drag and local barriers such as Peierls stresses. Once Peach-Koehler (PK) force is calculated, it is used to advance the

dislocation segment through a linear mobility law. Experimental data and atomistic simulations are used to get dislocation mobility.

$$F_s = F_{Peierls} + F_D + F_{Self} + F_{SF} + F_{External} + F_{Obstacle} + F_{image} \quad (11)$$

The dynamic dislocations is governed by a "Newtonian" equation of motion, consisting of an inertia term, damping term, and driving force arising from short-range and long-range interactions where the glide velocity v is calculated such that:

$$m_s \dot{v} + \frac{1}{M_s(T,p)} v = F_s \quad (12)$$

In the above equations, m_s is the effective dislocation segment mass, M_s is the dislocation mobility which could depend both on the temperature T and the pressure p (Zbib and de la Rubia 2002, Zbib, Shehadeh et al. 2003).

B. MDDP simulation set up

As mentioned in (Gurrutxaga-Lerma, Shehadeh et al. 2017), the simulation domain consists of a column of length L with square cross section h × h oriented in the [001]. The dimensions of the domain are$0.5\mu m \times 0.5\mu m \times 24\mu m$. The shockwave is generated by applying displacement-controlled boundary conditions on the upper surface. We confine the four sides to achieve the uniaxial strain condition involved in planar planes, and the lower surface is a reflective rigid boundary. The loading is in a way that a ramp wave of a particle velocity U_p is produced over a finite rise t_{rise}chosen based on the experimentally measured values of$\approx$ 1 ns.

Frank Read (FR) sources are randomly placed on the slip planes to act as a dislocation generation mechanism. The dislocation source length ranges between0.25 μm to $0.5\mu m$; resulting in an initial dislocation density is in the order of$10^{12} m^{-1}$. This initial value of the dislocation density is chosen to mimic the response of annealed crystals.

The input file to the program allows the user to specify the type of the crystal (BCC, FCC, and HCP) and to change the material constants (Young's modulus, shear modulus, Poisson's ratio, Mobility, burgers vector) with the temperature. Those values were taken from the literature (Gurrutxaga-Lerma, Shehadeh et al. 2017).

G. Simulation Setup

The simulation domain consists of a column of length L with square cross section h × horiented in the [001]. The dimensions of the domain are$0.57\mu m \times 0.57\mu m \times 11.4\mu m$. The shockwave is generated by applying displacement-controlled boundary conditions on the upper surface. We confine the four sides to achieve the uniaxial strain condition involved in planar planes, and the lower surface is a reflective rigid boundary. The loading is in a way that a ramp wave of a particle velocity U_p is produced over a finite rise t_{rise}chosen based on the experimentally measured values of$\approx$ 1 ns.

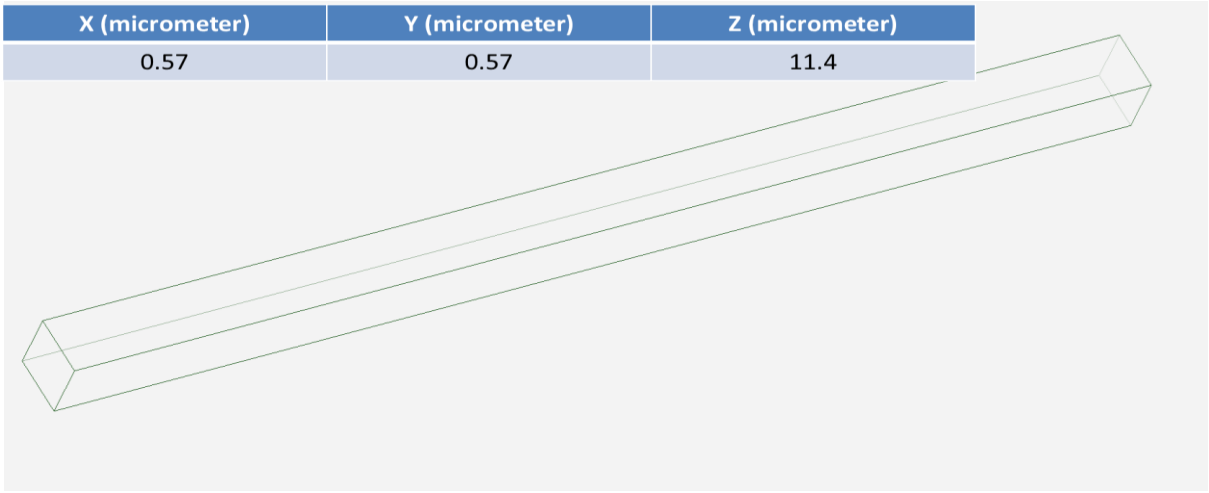


Figure 14: Simulation domain

Table 2: Simulated cases

Strain rate	Temperature	Rise time
1.01x10e8	**125K, 293K, 455K, 605K, 795K**	**1.5 ns**
3.95x10e7	**125K, 293K, 455K, 605K, 795K**	**0.75 ns**
2.11x10e6	**125K, 293K, 455K, 605K, 795K**	**0.75 ns**

Chapter III
Results and Discussions

A. Shock Wave Characteristics

Figure 16 displays the MDDP simulated wave profile of a shock generated at $10^7/s$ rate of deformation at 795 K deformation temperature. The wave history was recorded at the lower part of the sample. The longitudinal stress components of all finite elements at that location are averaged at each time step. Clearly, it takes the wave about 2 ns to travel the 8 μm distance during which the region stays in stress free state. Once the wave front arrives at the location of interest, the magnitude of the stress begins to increase until a maximum peak stress of 12GPa is attained over a finite rise time period of 1.5 ns. During the pressure buildup, we see that a ledge is formed on the wave front characterizing the dynamic yielding point. This ledge is a manifestation of stress relaxation that takes place due to the induced plasticity. It is worth noting that in order for the dynamic yielding point to form, a finite rise time must be included.

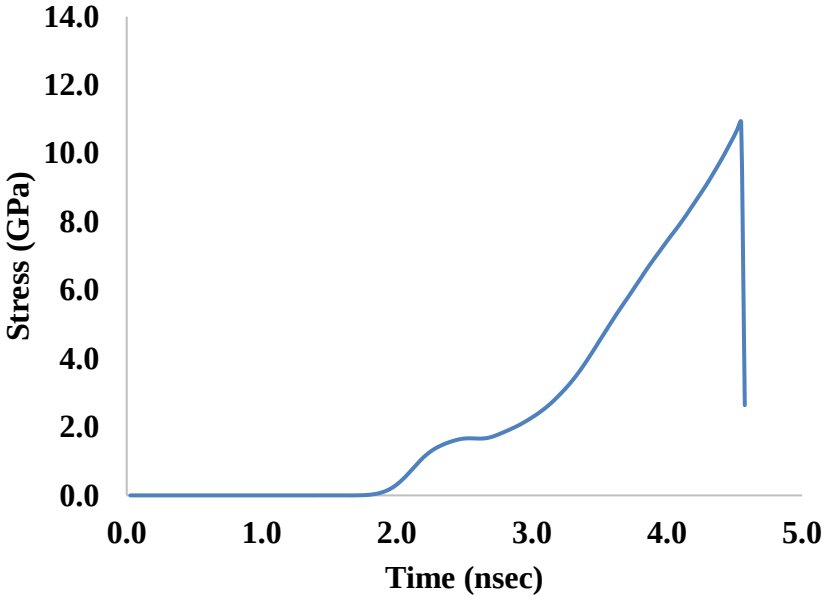


Figure 15: Shock front wave profile for a strain rate of 1.01×10^7/s and a temperature of 795K

B. Temperature Effect on the Dynamics Yielding

In shock experiments, measuring the decay in the dynamic yield during wave propagation is one of the direct ways to characterize flow stress dependence on strain rate (Zaretsky and Kanel 2012). In order to demonstrate MDDP capabilities in predicting the material's response, we have recorded the longitudinal wave history at sections taken on the upper, middle and lower parts of the simulation domain. Figure 16 displays the wave front at these three locations for a sample simulated at 10^7/s at 293 K. It is apparent that dynamic yielding point decays with the propagation distance which is attributed to the energy dissipated at the wave front as a result of dislocation-wave interaction.

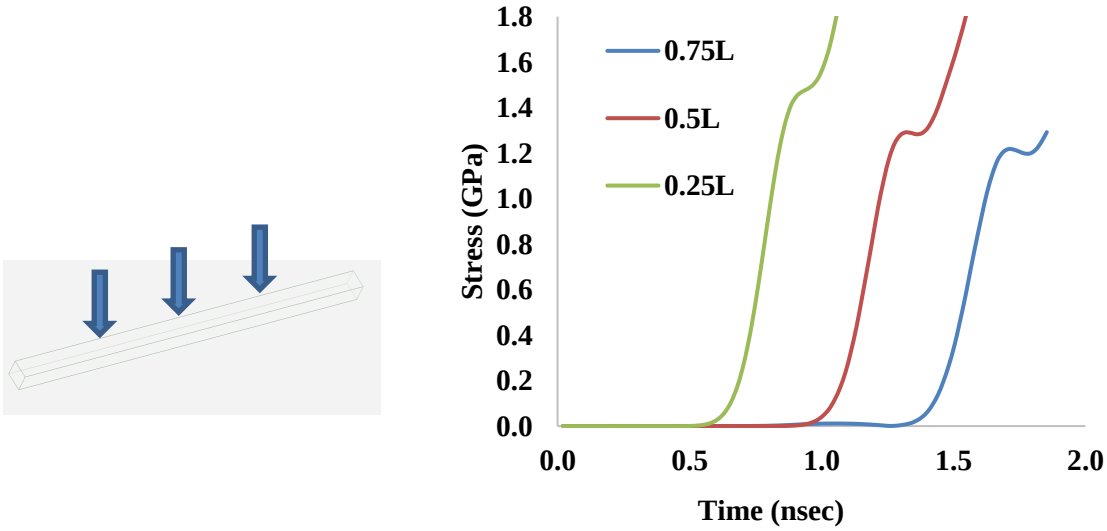


Figure 16: Elastic precursor decay for 1.01x10e7/s at 125K

For the same strain rate, we report in Figure 17, the magnitudes of the dynamic yielding point after the wave has travelled 9 µm at a temperature range of 125K to 800K. It is interesting to see that under this ultra-high strain rate; Al exhibits thermal hardening behavior which is in accordance with recent experimental findings (Zaretsky and Kanel 2012) (Gurrutxaga-Lerma, Shehadeh et al. 2017) and dislocation dynamics simulations (Gurrutxaga-Lerma, Shehadeh et al. 2017). This thermal hardening effect although counterintuitive, can be explained by the large increase in the dislocation drag force as the temperature increases which surpasses the temperature softening effect on the elastic properties and lattice friction (Chen, Asay et al. 2006).

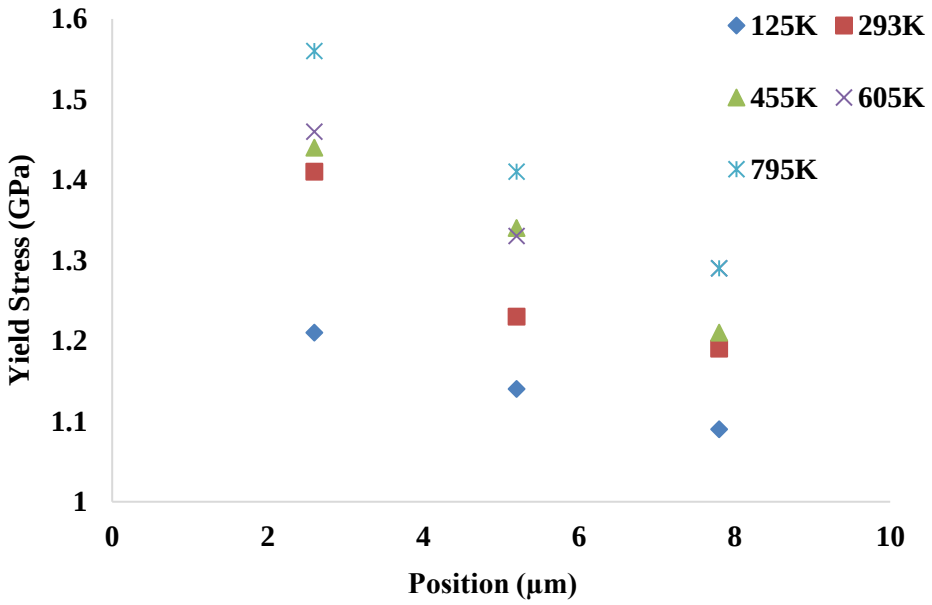


Figure 17: Elastic precursor decay for the 5 temperature values and the 3 strain rate values

Another observation is that the arrival time of the wave front is inversely proportional to the deformation temperature which may also partly contribute to the hardening effect. This is a consequence of the drop in the wave speed $c_l = \sqrt{\frac{2G(1+v)}{r}}$ resulting from the shear modulus softening as illustrated in figure18.

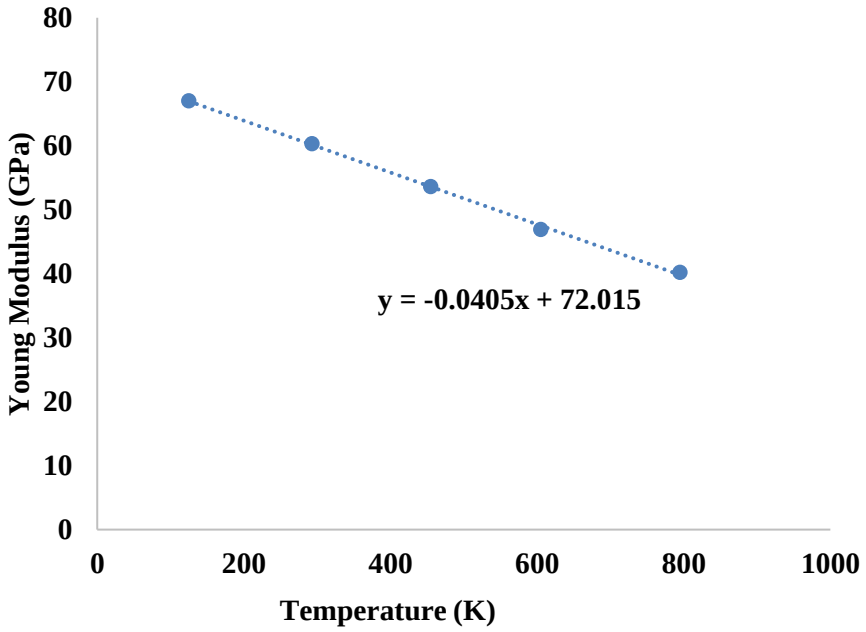


Figure 18: Magnitude of modulus of elasticity (Young's modulus) for the different temperatures investigated. Same values are obtained for different strain rates

As mentioned above, the elastic precursor decay is directly connected to the plastic dissipation process, and the rate of this decay provides important information on the flow stress-strain rate relationship as discussed in (Kanel 2012). Figure 19 shows MDDP generated data of the elastic precursor decay at various temperatures for a strain rate of$1.01 \times 10^7/s$. The thermal hardening effect is maintained at all positions where an increase in the yielding point with temperature at all travelled distances is seen. It is also observed that as the temperature increase, the rate of precursor decay becomes smoother.

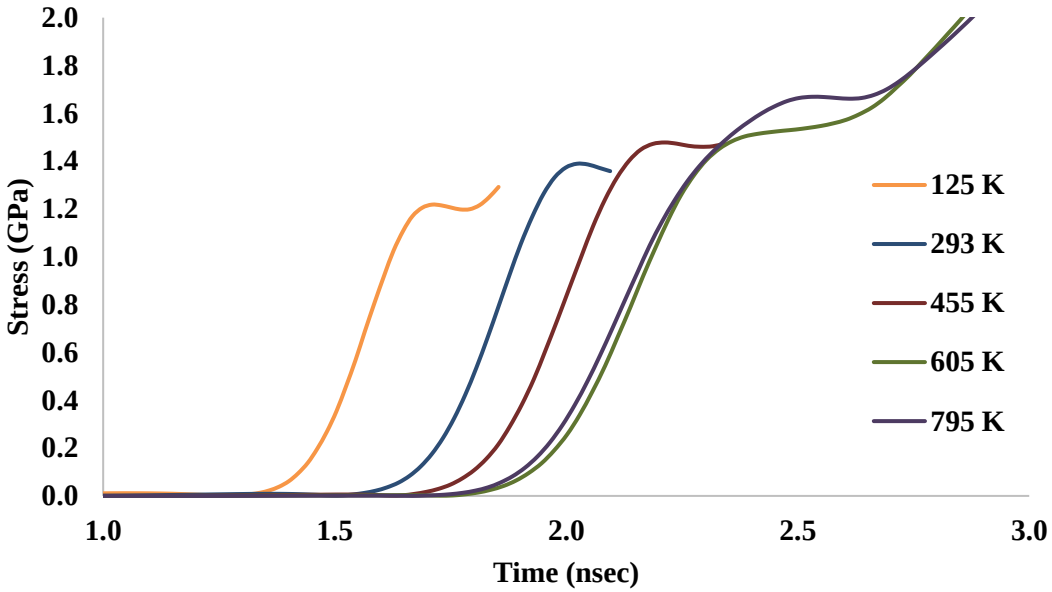


Figure 19: schematic of the shock waves profiles for FCC Al shocked at different temperatures with strain rate of$1.01 \times 10^7/s$. The peak of the elastic precursor or dynamic yield point increases with temperature for FCC Al. The shift among the curves shows the variation of wave's speeds with temperatures needed to be investigated

C. Constitutive Equations

One main driving force for lots of works is to obtain values for parameters to build constitutive equations of numerical simulation models (Kanel, Fortov et al. 2004). Using the curve fitting toolbox in MATLAB we curve fitted the different values we have for yield stresses, temperatures and the three positions in the specimen and got the following equations for the three strain rates values:

$$for\ a\ strain\ rate: 3.95 \times 10^{6} s^{-1}:$$

$$\sigma\,(T,x) = 2.174 - 0.2489T + 0.001798x + 0.0145T^{2} + 3.649 \times 10^{-5}Tx - 1.185 \times 10^{-6}x^{2} \quad (14)$$

$$for\ a\ strain\ rate: 1.01 \times 10^{7} s^{-1}:$$

$$\sigma\,(T,x) = 1.617 - 0.08656T + 7.008 \times 10^{-5}x + 0.00503T^{2} - 4.142 \times 10^{-5}Tx + 8.983 \times 10^{-7}T^{2} \quad (15)$$

$$for\ a\ strain\ rate: 1.8 \times 10^{8} s^{-1}:$$

$$\sigma\,(T,x) = 1.281 - 0.06372T + 0.00093x + 0.003698T^{2} - 2.989 \times 10^{-5}Tx - 4.277 \times 10^{-7}\,x^{2} \quad (16)$$

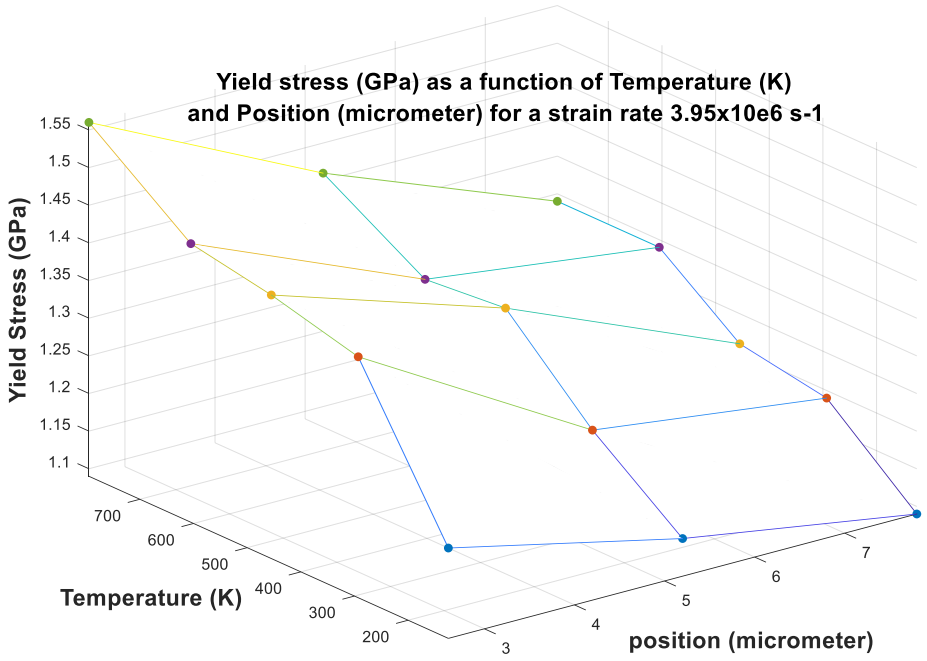


Figure 20: The curve fit of yield stress vs. Temperature and position for a strain rate of $3.95 \times 10^{6} s^{-1}$

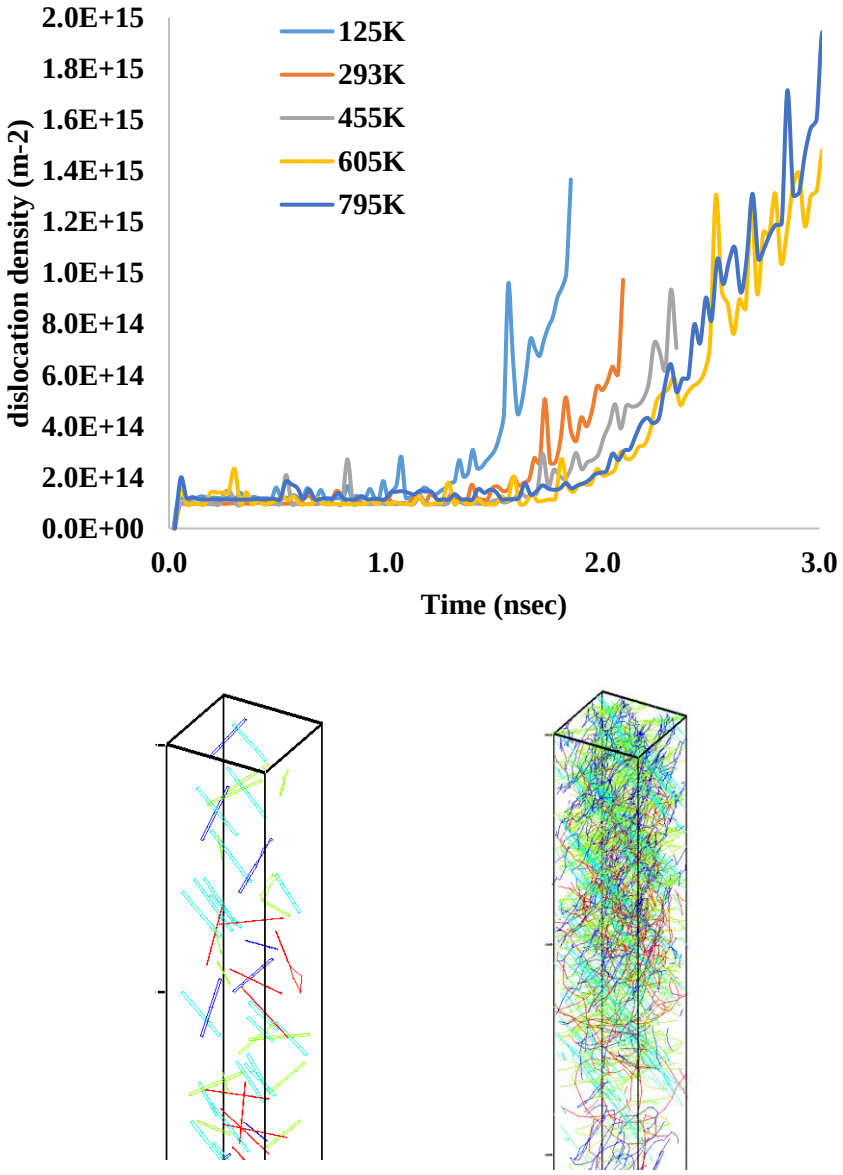


Figure 21: Dislocation density evolution at 1.01x10e7/s for the different temperatures

Chapter IV
Conclusion

We investigated the deformation mechanisms of Aluminum single crystals at three strain rates for a wide range of temperatures.

The report started in Chapter I with an overview of the different works in the literature that have been done around the field. Then, a good introduction on shock waves is provided, equation of state, and Rankine – Huguenot jump conditions. The first chapter ends with a rich introduction about dislocation theory, including their mechanisms of motion and deformation and nucleation.

In Chapter II, the methodology used in our study is briefly presented along with the simulation set up.

Chapter III presents the simulation results along with a detailed discussion including the shock wave characteristics, the temperature effect on the dynamic yielding, and the constitutive equations obtained using curve fitting toolbox in MATLAB.

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