Johns Hopkins Engineering

Applied Machine Learning for Mechanical Engineers

Machine Learning of Dislocation-Induced Stress Fields and Interaction Forces, Part 1, A

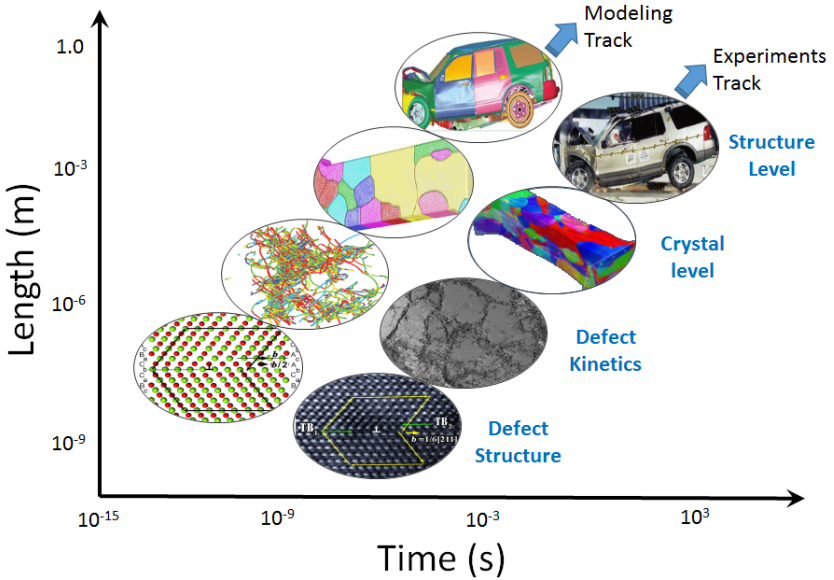
JOHNS HOPKINS
WHITING SCHOOL
of ENGINEERING

Simulations of Defects in Metals

- By the end of this lecture, you will be able to:
  - Describe multi-scale defects
  - Describe the bonds between atoms
  - Describe atomistic simulations
  - Describe dislocation
  - Describe edge dislocation stress field & force
  - Describe dislocation simulation challenges

Simulations of Defects in Metals

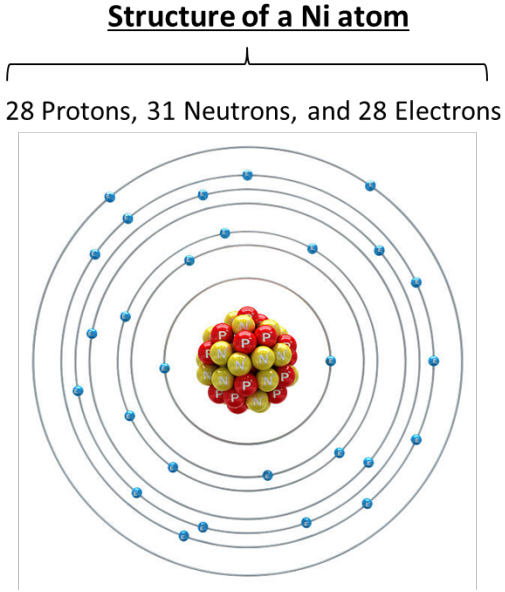
- Multi-Scale Defects
  - Material behavior: integration of multi-length and time scale phenomena



Courtesy of "Prof. Jaafar El-Awady"
https://me.jhu.edu/faculty/jaafar-el-awady/

Simulations of Defects in Metals

- Bonds Between Atoms
  - An atom is the basic unit (i.e., smallest constituent unit of an ordinary matter) of a chemical element
  - Atoms have a balanced electric charge
  - Electrons are present with different energies and it is convenient to consider these electrons surrounding the nucleus in energy shells
  - A common characteristic of metallic elements is they contain only one to three electrons in the outer shell
  - The bond between these electrons and the nucleus is relatively weak



Source: https://www.istockphoto.com/photo/niccolum-atom-on-a-white-background-gm502871592-82187499
Credit: generalfmv

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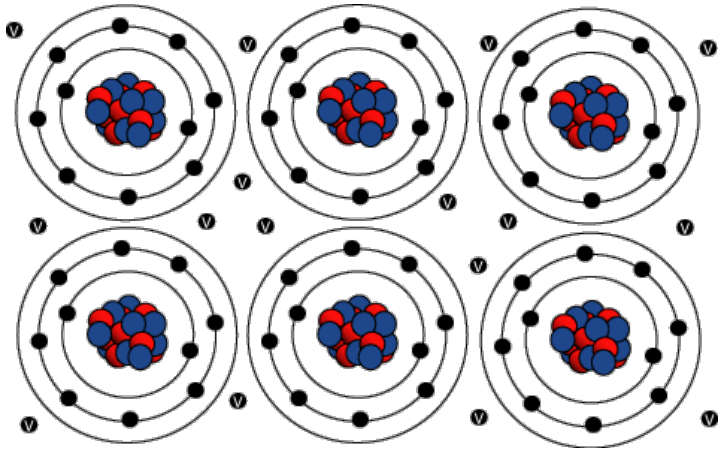
Simulations of Defects in Metals

- Bonds Between Atoms
  - Atoms will stay close together if they have a shared interest in one or more electrons.
  - Atoms are at their most stable when they have no partially-filled electron shells.
  - Thus, the electrons in the outmost shell tend to leave the atom and be shared between neighboring atoms in a common “electron cloud.”
  - Electrons in this cloud have considerable mobility and are able to conduct heat and electricity easily.



Source: https://www.nde-ed.org/EducationResources/CommunityCollege/Materials/Structure/metallic.htm

Courtesy of "Prof. Jaafar El-Awady"
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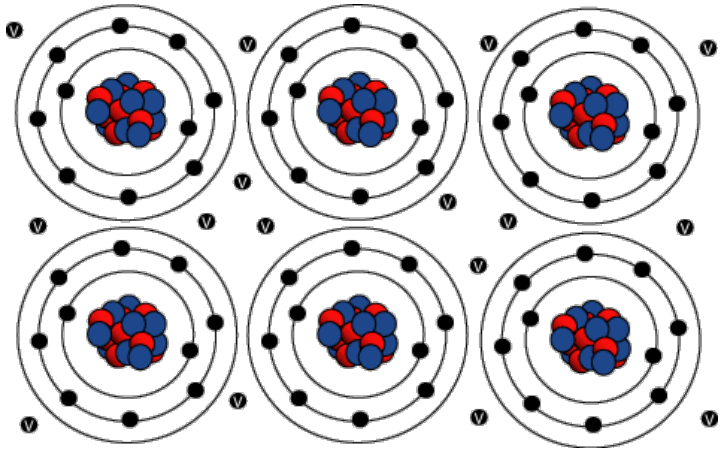
Simulations of Defects in Metals

- Bonds Between Atoms
  - The delocalized nature of the bonds makes it possible for the atoms to slide past each other when the metal is deformed instead of fracturing like glass or other brittle material.
  - The sharing of the electrons between atoms leads to the arrangement of atoms into a regular pattern (crystal structure) such that atoms are packed closely together to maximize the strength of the bonds



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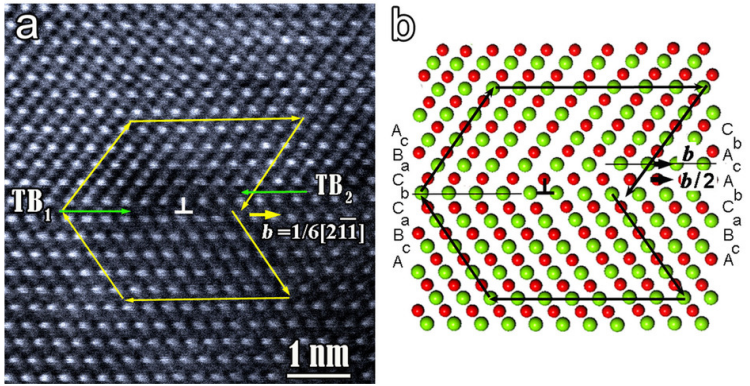
Simulations of Defects in Metals

- Atomistic Simulations
  - The goal of atomistic simulations is to model the collective behavior of atoms (i.e., the interactions between all atoms) forming a representative volume of a material.
  - Due to the large number of degree of freedom involved, several levels of coarse-graining can be utilized to model a relatively large material volume.



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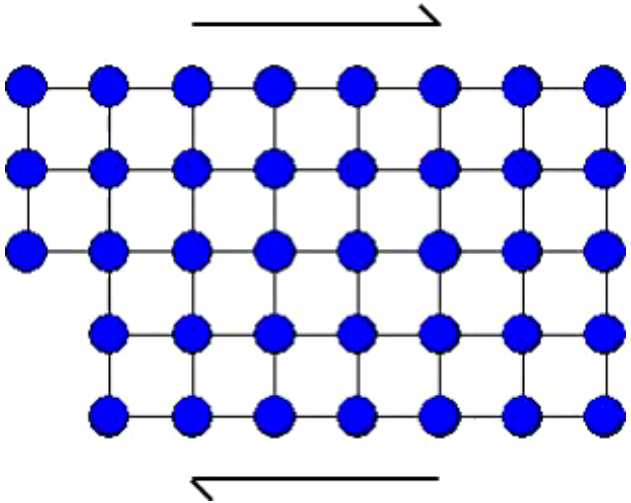
Simulations of Defects in Metals

- Dislocation
  - Atom slipping (dislocation glide)
  - The delocalized nature of the bonds makes it possible for the atoms to slide past each other when the metal is deformed instead of fracturing like glass or other brittle material.
  - Symbol ⊥ represents dislocation in the video.
  - The horizontal line represents what is called the “slip plane,” the plane that atoms are slipping through.
  - Burgers' direction is referred to as the direction that symbol ⊥ is moving in the video.
  - The vertical line represents what is called as the “extra half-plane.”



Source: https://youtu.be/kk2oOxSDQ7U

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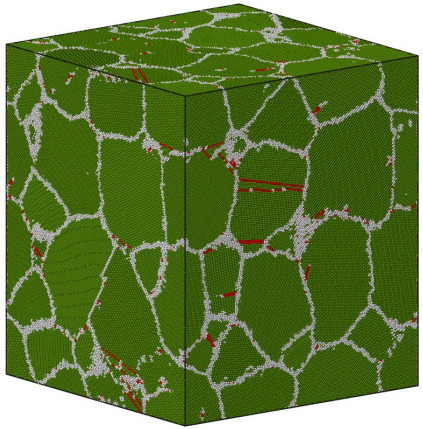
Simulations of Defects in Metals

- Dislocation
  - Atom slipping (dislocation glide)
  - 3D course-grain scale
  - Dislocation extraction algorithm



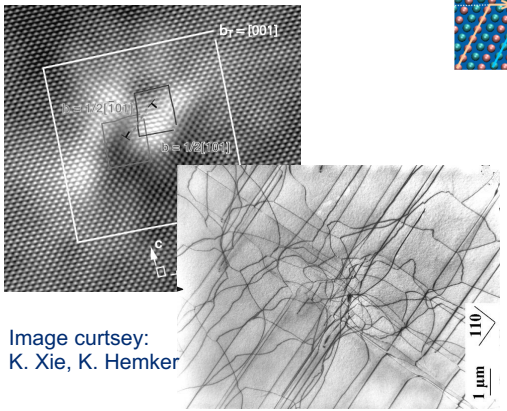
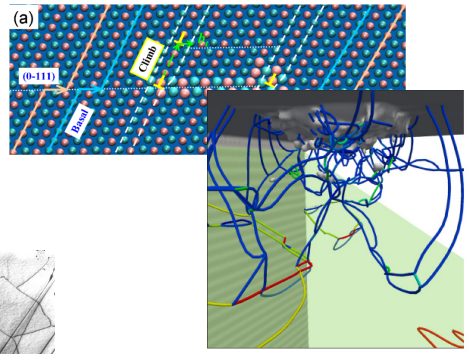


Image curtsey:
K. Xie, K. Hemker

Atomistic Simulations



Discrete Dislocation Dynamics Simulations

Source: Stukowski, A. (2012). Structure identification methods for atomistic simulations of crystalline materials. Modelling and Simulation in Materials Science and Engineering, 20(4), 045021

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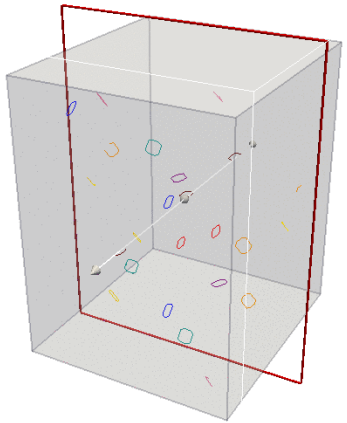
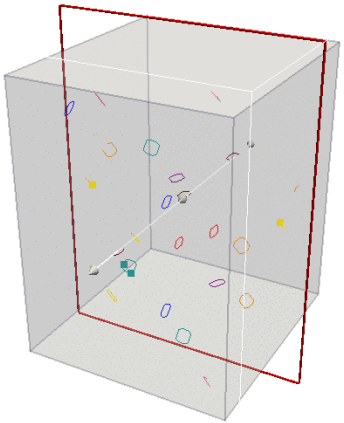
Simulations of Defects in Metals

- Dislocation
  - 3D to 2D representation of dislocations

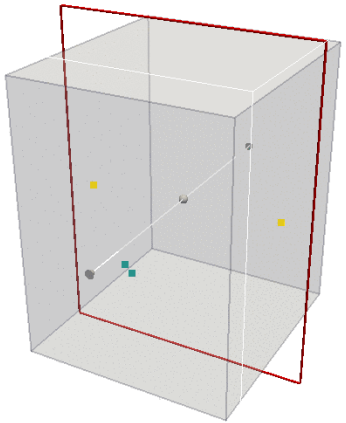
3D Dislocations Evolving



Intersection with Plane



2D Representation



Source: http://umet.univ-lille1.fr/Projets/RheoMan/en/to-learn-more-about/dislocation-dynamics.php

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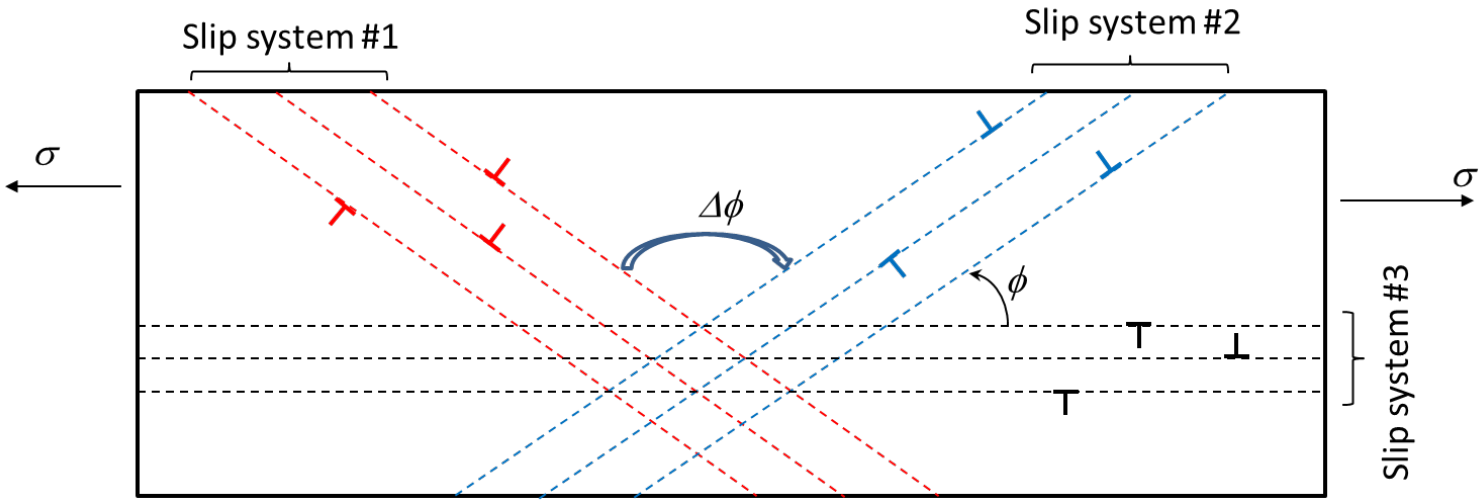
Simulations of Defects in Metals

- Dislocation
  - 2D representation of dislocations



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Simulations of Defects in Metals

- Edge Dislocation Stress Field & Force
  - Stress in 2D

Stress Field:

$$\sigma_{xx} = -\frac{Gb}{2\pi(1-\nu)}\cdot\frac{y(3x^2+y^2)}{(x^2+y^2)^2}$$

$$\sigma_{yy} = \frac{Gb}{2\pi(1-\nu)}\cdot\frac{y(x^2-y^2)}{(x^2+y^2)^2}$$

$$\sigma_{xy} = -\frac{Gb}{2\pi(1-\nu)}\cdot\frac{x(x^2-y^2)}{(x^2+y^2)^2}$$

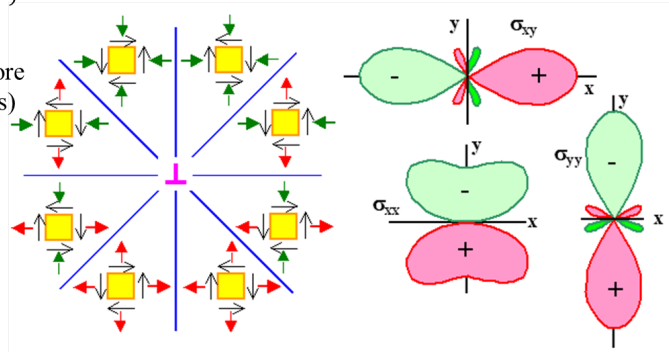
$$\sigma_{zz} = \nu(\sigma_{xx}+\sigma_{yy})$$

Notice the singularity at the core (linear theory of elasticity fails)

Displacement Field:

$$u_x = \frac{-b}{2\pi}\left[\tan^{-1}\left(\frac{y}{x}\right)+\frac{1}{2(1-\nu)}\frac{xy}{(x^2+y^2)}\right]$$

$$u_y = \frac{b}{8\pi(1-\nu)}\left[(1-2\nu)\ln(x^2+y^2)+\frac{(x^2-y^2)}{(x^2+y^2)}\right]$$



Source: https://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/illustr/i5_2_1.html

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Simulations of Defects in Metals

- Edge Dislocation Stress Field & Force
  - Force
    - If the stress field is known at the position at which the dislocation is located, the force on the dislocation at position $\mathbf{R}$ can be computed from the Peach-Koehler relationship

$$\mathbf{F}_i(\mathbf{R}) = (\boldsymbol{\sigma}(\mathbf{R}) \cdot \mathbf{b}_i) \times \mathbf{t}_i(\mathbf{R})$$

where $\boldsymbol{\sigma}(\mathbf{R})$ is the stress tensor at position $\mathbf{R}$, $\mathbf{b}_i$ is the Burgers vector of the dislocation, and $\mathbf{t}_i(\mathbf{R})$ is the tangent to the dislocation at position $\mathbf{R}$.

Source: https://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/illustr/i5_2_1.html

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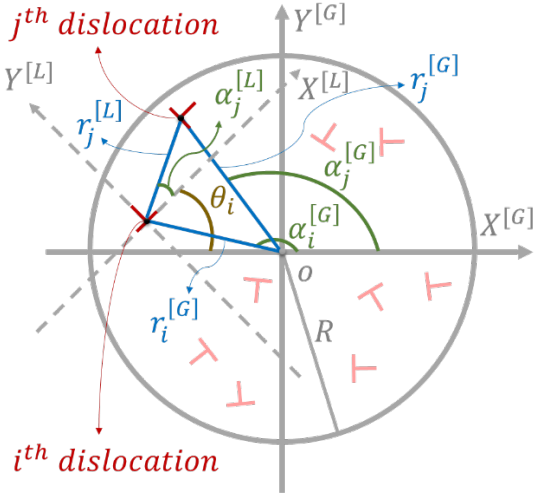
Simulations of Defects in Metals

- Dislocation simulation challenges
  - Suppose we have a theoretical circular two-dimensional (2D) domain having radius R and containing N randomly oriented infinite long edge dislocations.
  - To compute the force on a dislocation, we need the stress imposed on that dislocation from every other dislocation. That is N-1 stress calculations.
  - We have N dislocations, then N force calculations are needed.
  - So, the total number of calculations is N(N-1) calculations at each time. Once the forces are computed, each dislocation will have a new position. Then another N(N-1) calculations are required for the next step (simulating the evolve).
  - Simulation of dislocation evolving is very time-consuming.
  - This is just 2D. 3D version would be more time-consuming.



Source: Rafiei, M. H., Gu, Y., & El-Awady, J. A. (2020). Machine Learning of Dislocation-Induced Stress Fields and Interaction Forces. JOM, 1-13.

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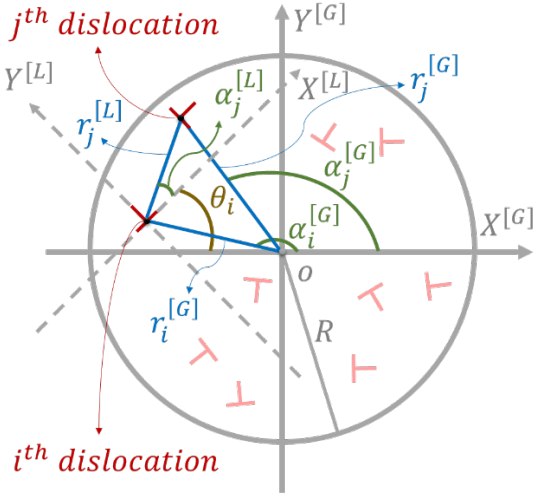
Simulations of Defects in Metals

- Dislocation simulation challenges
  - Machine learning techniques are capable of accelerating materials simulations including dislocation simulation
  - Machine learning techniques require an appropriate repository for training and evaluation
  - Once trained, the testing is not that time-consuming
  - There is a trade-off between machine learning accuracy and acceleration.
  - The type and architecture of the machine learning technique are keys in discovering a fast and accurate machine learning technique.
  - In this module, our focus is on accuracy only.



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Simulations of Defects in Metals

- In this lecture, you learned about:
  - Multi-scale defects
  - The bonds between atoms
  - Atomistic simulations
  - Dislocations
  - Edge dislocation stress field & force
  - Dislocation simulation challenges

- In the next lecture, we will formulate the machine learning dislocation model of Rafiei et al. (2020).

Rafiei, M. H., Gu, Y., & El-Awady, J. A. (2020). Machine Learning of Dislocation-Induced Stress Fields and Interaction Forces. JOM, 1-13.