RADIATION DAMAGE IN MATERIALS

PARTICLES WITH KINETIC ENERGIES ABOVE THERMAL ENERGIES

$E_{KIN} > 1\,eV$ EXIST FROM COSMIC RAYS, NORM. DECAY,

+ MAN-MADE DEVICES, ACCELERATORS FOR MEDICINE,

IRRADIATION, CANCER TREATMENT ETC., DEGRADATION OF MATERIALS NEEDS TO BE UNDERSTOOD

NUCLEAR REACTORS ARE KEY CUSTOMERS

- CONSEQUENCE OF HIGH ENERGY PARTICLE INTERACTION WITH MATERIALS IS THE FORMATION OF LATTICE DEFECTS.

  (ADDITIONALLY THERE IS PRODUCTION OF PHONONS, PLASMONS, SECONDARY e^- + PHOTONS, HEATING)

THIS CONSEQUENCE IS REASON RADIATION HAS DETRIMENTAL + BENEFICIAL EFFECTS ON MATERIALS.

IN A CRYSTAL AN ATOM CAN BE KICKED OUT OF ITS LATTICE SITE, CREATING AN INTERSTITIAL SITE.

MUCH MORE COMPLICATED DEFECTS CAN BE FORMED.

- DEFECT CLUSTERS
- AMORPHOUS ZONES
- DISLOCATION LOOPS

SURFACE DEFECTS
- CRATERS
- RIPPLES

- DAMAGE PRODUCTION MECHANISMS CAN IN MOST CASES BE DIVIDE INTO 2 CATEGORIES BY TIME SCALE
  - PRIMARY DAMAGE

PRIMARY DAMAGE IS FORMED IMMEDIATELY THE PARTICLE IMPACTS BY ATOMIC COLLISION PROCESS & STRONG MATERIAL HEATING CAUSED IS FAR FROM THERMODYNAMIC EQUILIBRIUM.

TIME SCALE:

$$\tau \sim 0.1 \rightarrow 1\,ps.$$

SUBSEQUENT THERMALIZATION ~

$$\tau \; 1 \rightarrow 10\,ps$$

"ATHERMAL" IN THAT THERMALLY ACTIVATED PROCESSES ARE NOT SIGNIFICANT

LONG-TERM SCALE DAMAGE

TYPICALLY REQUIRE THERMAL ACTIVATION & LONG TIME SCALES RANGING FROM 10^{-9} sec → YEARS

DPA = DISPLACEMENT-PER-ATOM

INSPIRED BY ORIGINAL IDEAS OF RADIATION DAMAGE LEADING TO THE PRODUCTION OF PRIMARY POINT DEFECTS, BUT HAS BEEN REFINED.

CONCEPT IS THAT ENERGETIC PARTICLES TRAVEL MOSTLY STRAIGHT IN MATERIAL, & OCCASIONALLY COLLIDES STRONGLY IN A BINARY COLLISION & IMPARTS ENERGY TO A LATTICE ATOM.

FOR γ, n & e^- THIS IS A GOOD APPROXIMATION DUE TO THEIR SMALL CROSS SECTION FOR COLLISION

- IONS + ATOMIC RECOILS MAY COLLIDE WITH SEVERAL NEAREST-NEIGHBOR ATOMS MAKING THIS A MANY BODY AS OPPOSED TO BINARY IN NATURE.
~~THIS THEN IS CALLED THEN~~

- THE MULTIPLE SIMULTANEOUS COLLISIONS CAN BE DESCRIBED AS A "DISPLACEMENT SPIKE" OR "HEAT SPIKE"

- FOR A BINARY COLLISION IT IS OBVIOUS THAT IF ENERGY IMPARTED TO THE LATTICE ATOM IS LESS THAN THE COHESIVE ENERGY OF AN ATOM IN THE LATTICE, IT WILL NOT LEAVE THE SITE + NO DAMAGE DONE.

- IF ENERGY IMPARTED IS ORDERS OF MAGNITUDE HIGHER THAN THE COHESIVE ENERGY, THE ATOM ~~CAN BECOME~~ BECOMES A RECOIL ATOM THAT MOVES THROUGH THE MATERIAL PRODUCING MORE DEFECTS.

$$T_D = F_{D,n} = E_0 - F_{D,e}$$

- E_0: INITIAL ENERGY
- $F_{D,e}$: ENERGY LOST TO ELECTRONIC STOPPING POWER ← L.E.T.
- T_D: TOTAL ENERGY AVAILABLE TO DO DAMAGE
- $F_{D,n}$: "NON-IONIZING" ENER LOSS ~~R~~NIEL

- E_d = THRESHOLD DISPLACEMENT ENERGY

  HIGHER THAN THE COHESIVE ENERGY
  TYPICALLY 5eV/atom IN TYPICAL LIMD SOLIDS

- SIMULATIONS DEVELOPED ~~TO~~ BASED ON BINARY COLLISION APPROXIMATION (BCA) HAS LEAD TO THE GENERALLY ACCEPTED NRT (FOR THE AUTHORS) EQUATION.

$$N_d(T_d) = \begin{bmatrix} 0, & T_d < E_d \\ 1, & E_d < T_d < 2E_d/0.8 \\ \frac{0.8T_d}{2E_d}, & \frac{2E_d}{0.8} < T_d < \infty \end{bmatrix}$$

0.8 IS FACTOR DETERMINED BY SIMULATIONS.

∴ THIS EQN IS THE BASIC EQN TO CALCULATE THE NUMBER OF DISPLACED ATOM IS ANY MATERIAL FOR WHICH E_d IS KNOWN & T_d CAN BE CALCULATED.

- IF N_p IS NORMALIZED TO THE # OF ATOMS IN A GIVEN VOLUME THEN ONE OBTAINS THE UNITLESS QUANTITY DPA

$$\text{DPA} \equiv \text{DISP PER ATOM} = \frac{\#\text{ OF DISPLACED ATOMS FROM NRT EQN}}{\#\text{ OF MATERIAL ATOMS IN SAME VOLUME}}$$

WHICH SIMPLY GIVES THE DEFECT CONCENTRATIONS OF PRIMARY VACANCIES + INTERSTITIAL IN THE MATERIAL.

AKA $C_V = C_i = C_{\text{FRENKEL PAIR}}$

- DPA CONCEPT IS WIDELY USED IN ESTIMATING AMOUNT OF RADIATION DAMAGE IN MATERIALS.
  - > MORE TELLING THAN SAY $10\ kJ/m^3$,
    BUT 0.01 DPA COMMUNICATES 1 ATOM IN 200 HAS BEEN DISPLACED / DAMAGED,
  - > ALLOWS FOR SCALING ~~BETWEEN~~ DOSES OR FLUENCES BETWEEN DIFFERENT KINDS OF IRRADIATIONS

INDUSTRY STANDARD

IT IS STRONGLY RECOMMENDED TO USE DPA IN NEUTRON TRANSPORT CALCULATIONS TO MAKE TRANSFERRABLE INTERPRETATION OF DIFFERENT KINDS OF NEUTRON IRRADIATION.

ASTM STANDARD E693-94 DEFINES HOW THESE CALCULATIONS SHOULD BE DONE IN Fe

LET US UNDERSTAND E_d ~~BETTER~~ BETTER

VELOCITY OF A RECOIL IN A LATTICE IS MUCH LARGER THAN THE CONVENTIONAL THERMAL VELOCITY.

30eV RECOIL HAS KIN. ENERGY 1000x AVG THERMAL VELOCITY 0.03eV, ~~[illegible]~~

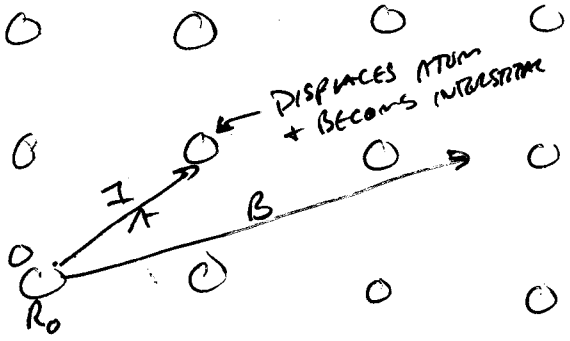
HENCE VELOCITY $\sqrt{1000} \approx 30\times$ HIGHER.

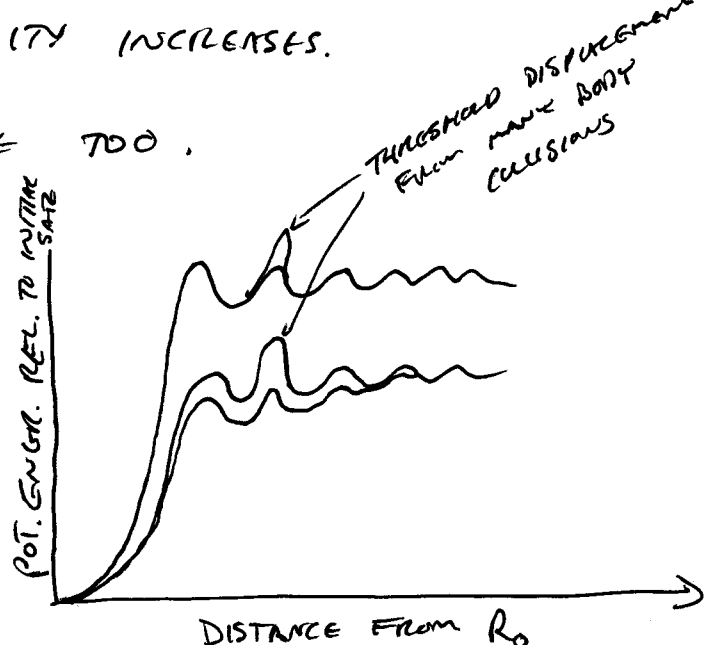
- THERE IS NOT A SINGLE THRESHOLD ~~[illegible]~~ DISPLACEMENT ENERGY, ~~BUT [illegible]~~ EACH CRYSTAL HAS ITS OWN DUE TO CRYSTAL ANISOTROPY;

  EACH ATOM HAS SOME KINETIC ENERGY, DISTRIBUTED ACCORDING TO MAXWELL-BOLTZMANN DISTRIBUTION.

1. IF THERMAL VELOCITY HAPPENS TO BE IN DIRECTION OF THE RECOIL ENERGY, DAMAGE PRODUCTION PROBABILITY INCREASES.

2. THE REVERS IS TRUE TOO.





WHILE THRESHOLD DISPLACEMENT ENERGIES HAVE BEEN STUDIED EXTENSIVELY BY M.S.E. & MECH E. IN SIMULATION & EXPERIMENTALLY, THERE ARE STILL UNCERTAINTIES FOR SEVERAL TECHNOLOGICALLY IMPORTANT MATERIALS.

PERHAPS THE MOST FRUSTRATING IS Fe

THERE IS NO EXPERIMENTAL VALUE FOR THE AVG THRESHOLD. THERE ARE HUGE VARIATIONS

SILICON ALSO LARGE VARIATION.

↳ BECOMES A QM PROBLEM USING DENSITY FUNCTIONAL THEORY (DFT)

CALCULATING DPA IN METALS (1 INCIDENT PARTICLE)

REQUIRES KNOWLEDGE OF NEUTRON FLUX ENERGY SPECTRUM & TIME

$$\phi(E,t)$$

ATOMIC DISPLACEMENT CROSS SECTION FOR PARTICULAR MATERIAL, σ_d, WHICH IS ALSO A FUNCTION OF ENERGY: $E \rightarrow \sigma_d(E)$

THINK OF AS EFFECTIVE AREA, THAT IF CROSSED BY 1 WILL LEAD TO DISPLACEMENT.

$$\frac{dpa}{s} = \int_0^\infty dE\, \sigma_d(E)\, \phi(E,t)$$

TOTAL AMOUNT OF DPA

$$dpa = \int_0^{t_e} dt \int_0^{\infty} dE\, \sigma_d(E)\, \phi(E,t)$$

CONVENIENT TO DECOMPOSE THE NEUTRON FLUX INTO A FACTOR THAT CARRIES THE TIME DEPENDENCE & A NORMALIZED FLUX SPECTRUM, WHICH WOULD EQUAL UNITY WHEN INTEGRATED OVER ENERGY $\psi(E,t)$

$$dpa = \int_0^{t_e} dt\, \phi_{tot}(t) \int_0^{\infty} dE\, \sigma_d(E)\, \psi(E,t)$$

IF WE CAN CONSIDE FLUX SPECTRUM TO BE CONSTANT OVER TIME

$$dpa = t_e\, \phi_{tot} \int_0^{\infty} dE\, \sigma_d(E)\, \psi(E)$$

ATOMIC DISPLACEMENT CROSS SECTION IS DETERMINED BY WEIGHING RESULTS OF 3 PROCESSES

1. NUCLEAR REACTION BETWEEN INCIDENT NEUTRON & THE NUCLEUS OF THE ATOM, & RELAVENT TRANSFER OF ENERGY FROM THE NEUTRON (E) TO NUCLEUS (T).
2. LOSS OF ENERGY ACQUIRED BY NUCLEUS VIA INTERACTION WITH e^- OF THE SYSTEM $E(T \rightarrow T_d)$
3. ACTUAL DISPLACEMENTS BASED ON EMPIRICAL DATA

OPTIONAL

STRONG EXPERIMENTAL & SIMULATION EVIDENCE THAT DAMAGE DOES NOT INCREASE LINEARLY WITH DEPOSITED DOSE.

THIS IS QUANTIFIED BY THE DAMAGE EFFICIENCY PARAMETER ξ

$$\xi \equiv \frac{\text{ACTUAL DAMAGE}}{\text{NRT PREDICTED DAMAGE.}}$$

EMPIRICAL EXPERIMENTS SHOW DAMAGE PRODUCED BY IONS OR RECOILS WITH ENERGIES WELL ABOVE THE THRESHOLD DISPLACEMENT ENERGY PRODUCED SUBSTANTIALLY LESS DAMAGE THAN EXPECTED BY NRT EQN.

INSIGHT TO THIS COMES FROM SOPHISTICATED SIMULATION.

- A SET OF BALLISTIC COLLISIONS LEADS TO MAJOR PRODUCTION OF DISPLACED ATOMS. (WHICH IS CLOSE TO NRT PREDICTION) ~200 fs

- HOWEVER, AFTER THIS THE CASCADE BECOMES A HEAT SPIKE (THERMAL SPIKE)

  "DENSE REGION OF MANY BODY ATOMIC COLLISIONS THAT IS UNDER DENSE IN THE MIDDLE & OVERDENSE ON THE PERIPERY

  ~1 ps BEHAVES LIKE THERMODYNAMIC SYSTEM.

WITH TEMPERATURES ON ORDER OF 10,000 K

NOTE WORTHY 3 LATTICE VIBRATIONS ~ 1 ps

HEAT SPIKE DURATION IS ~ 10 ps

↳ COOLING DOWN OF THE HEAT SPIKE CAN RECRYSTALIZE, WHICH TENDS TO PRODUCE A PERFECT CRYSTAL.

THUS MANY OF THE DISPLACED ATOMS REGENERATE DURING THE THERMODYNAMIC PHASE.

WHICH EXPLAINS DAMAGE EFFICIENCIES BELOW 1.

SINCE THIS RECOVERY DOES NOT REQUIRE THERMALLY ACTIVATED MIGRATIONS THIS RECOMBINATION IS CALLED ATHERMAL (IT WOULD HAPPEN IF SAMPLE WERE AT 0K)

SO WHY IS $\xi \neq 0$. FOR ALL INTERACTIONS?

↳ INTERSTITIAL & CLUSTERS REMAIN AT OUTSKIRTS, OF HEAT SPIKE REGION.

TEMPERATURE PROFILE LEADS TO PROBABILITY OF RECOMBINATION

$P = e^{E_F/kT}$ ← TEMP AT RECRYSTALIZATION FRONT.
↑ VACANCY FORMATION ENERGY