Estimate of Radiation Damage Using the Stopping and Range of Ions in Matter

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Abstract

Displacement theory describes the process wherein a neutron collides with an atom within a material, imparting energy to it, denoted as T

This collision is often referred to as the Primary Knock-on Atom (PKA). If the energy of the PKA is sufficiently high, it can trigger additional displacements, leading to a cascade effect known as Secondary Knock-on Atoms and beyond.
This process results in the creation of numerous defects within the material, including interstitials
we need to make comparison between the system full damage and quick calculation according to change of energy , light or heavy particles ,number of particles

The NRT modified KP model

The Norgett, Robinson, and Torrens (NRT) model, introduced in 1975, represents a refinement of the original Kinchin-Pease (KP) model and remains widely employed in the contemporary assessment of radiation damage in nuclear materials.

This modification addresses specific assumptions within the KP model:

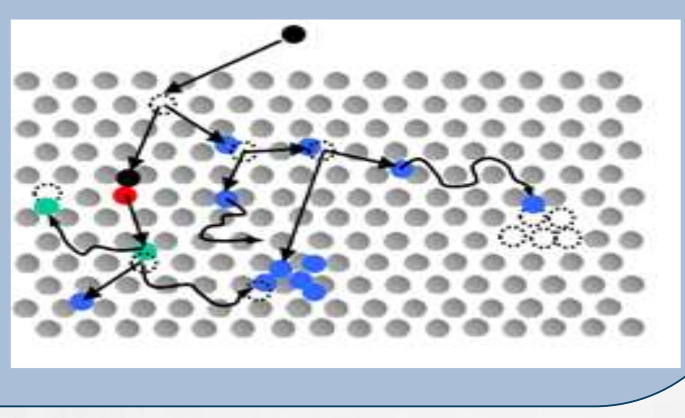
- Adjustment to the energy loss mechanism involving the electronic system through the introduction of a cutoff threshold Ec
- If the Primary Knock-on Atom (PKA) possesses energy exceeding this threshold, further displacements cease.

Adoption of the hard-sphere model for the energy transfer cross-section. According to this model, atoms are treated as rigid spheres incapable of spatial overlap, enhancing the accuracy of the energy transfer estimation.

Introduction

It is essential to predict/simulate:
- Defects created by neutron/ion irradiation
- Long-term evolution of defects and impurities
•Defects formed during cascade are required as input. However, high-energy neutrons generate PKA with high energy (~MeV), which implies a very large amount of displacements
Neutron irradiation induces Elastic and nuclear reaction. The displacement of ions (PKA spectrum) are generated with both Inelastic elastic and inelastic reactions, although the elastic reaction contribute, more or less, in more than of a 90 %, depending on the isotope analyze.
Heavy Ion (PKA spectrum) irradiation mainly induces elastic reactions producing displacements damage
a)Neutron/Ion irradiation produces different
•It is essential to predict/simulate:
- Defects created by neutron/ion irradiation
- Long-term evolution of defects and impurities

types of defects: I, V, He, H, clusters…
After they are created, defects can:
-Migrate, Agglomeration ,recombination



Methodology

SRIM/TRIM ANALYSIS:
Vacancies and Damage calculation
SRIM-2013 code has used to calculate the total vacancy by difference energies for proton and fe irradiation damage. The option of this code was calculated by using Ion Distribution and Quick Calculation of Damage (Kinchin-Pease model). Calculations were for H and fe ions implantation into zr and fe for a range of H ion energies using 50kev , 2 and 10 MeV
of PKA. The threshold displacement energy used in the calculations was 40 ,35,25 eV for Fe and zr based on ASTM E521 Standard and the lattice binding energy was set at 0 and 3 ev. Then, the incident ion was changed for 2000,5000,10000 ions and there are cases are used 12000 and15000 ions. At the end, the data has found in the "vacancy.txt" output files, which were detailing the number of vacancies created for ions and recoils. Fig. 2 shows SRIM calculation of vacancy creation cause H(10Mev) into zr and fe(2 Mev) into fe .
In the case of 10 MeV H into zr with binding energy 0 and 3 ev displacement energy for zr (40 ev)

Displacement energy (Ed) :

is a crucial parameter in nuclear materials, particularly in the nuclear industry. The table provides details regarding various metals commonly employed in nuclear applications, listing their respective minimum and average displacement energies (Ed)

In DPA (Displacement per Atom) calculations, a single average displacement energy (Ed) is utilized. This average is derived from the mean of specific values pertaining to crystallographic characteristics.

Metal	E_{dmin} /eV	E_d/eV
Al	16	25
Ti	19	30
Cu	19	30
Zr	21	40
W	40	90
Ta	34	90
Fe	20	40
Stainless steel		40

comparison between different binding energies and different energy displacements

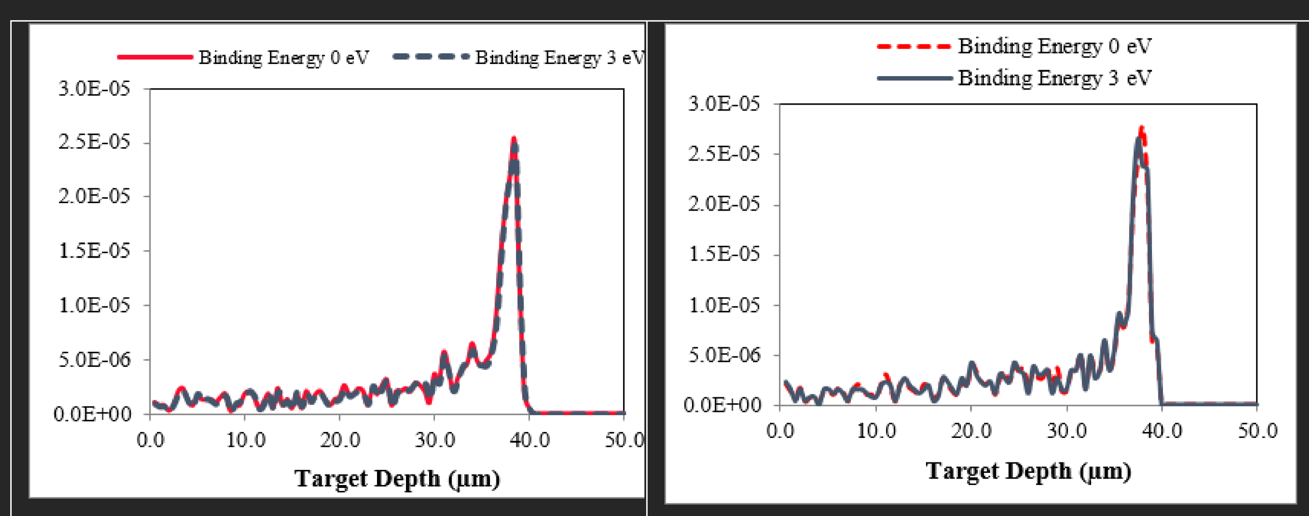
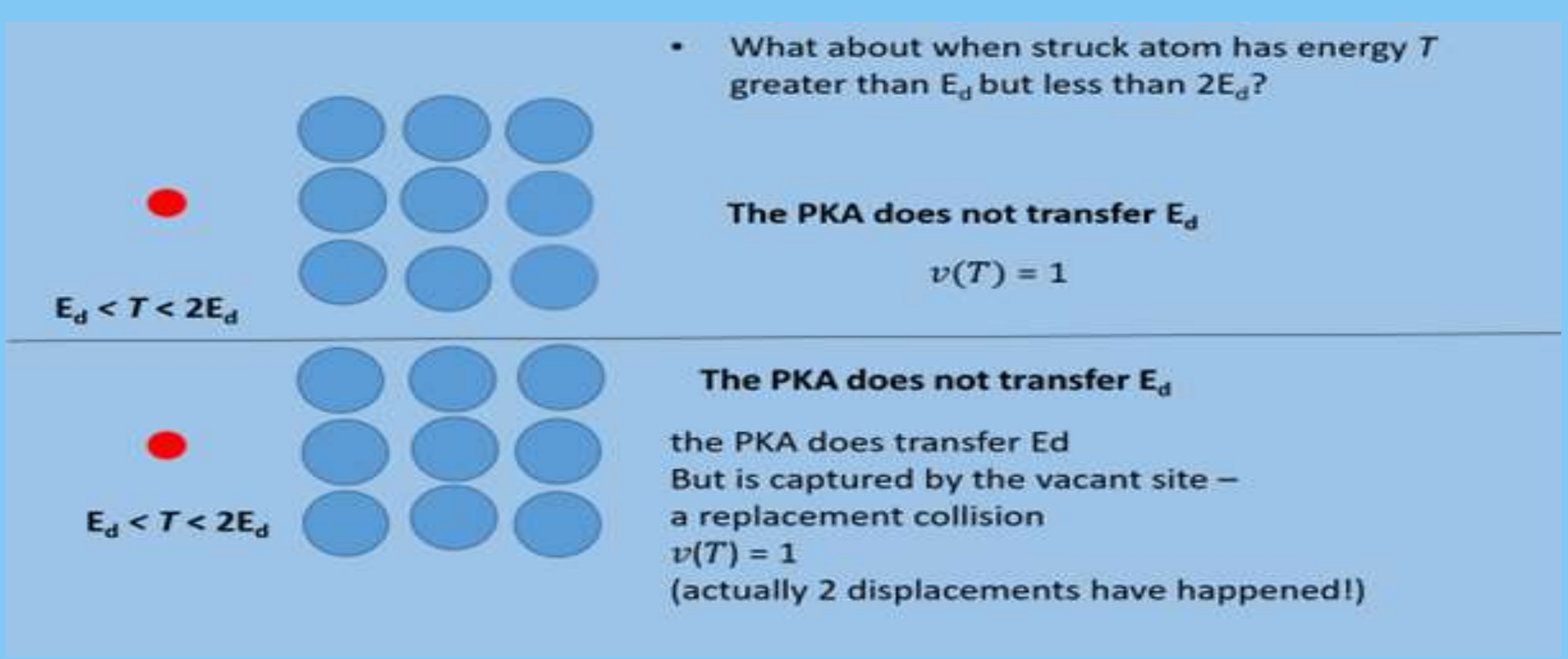


Fig.1.10 MeV H ions in Zr target (K-P mode)　Fig.2. 10 MeV H ions in Zr target (F-C mode)

The Kinchin and Pease (KP) model



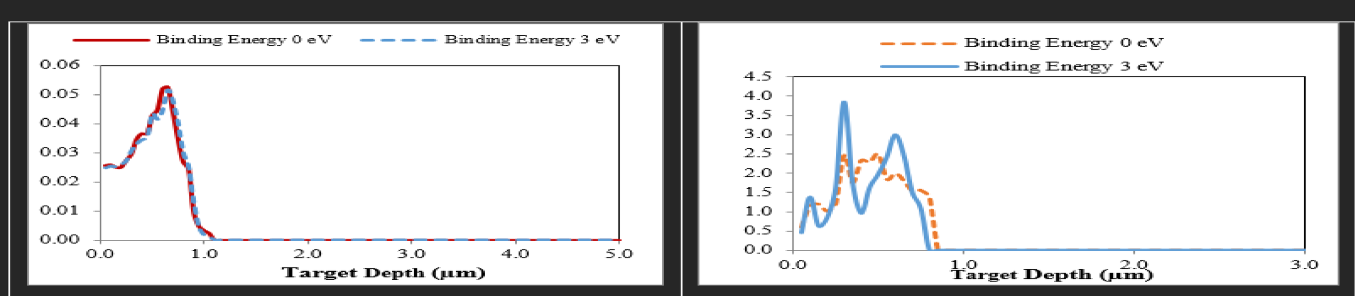


Fig.3. 2 MeV Fe ions in Fe Target K-P mode)　Fig.4.2 MeV Fe ions in Fe Target F-C mode)

Displacement energy

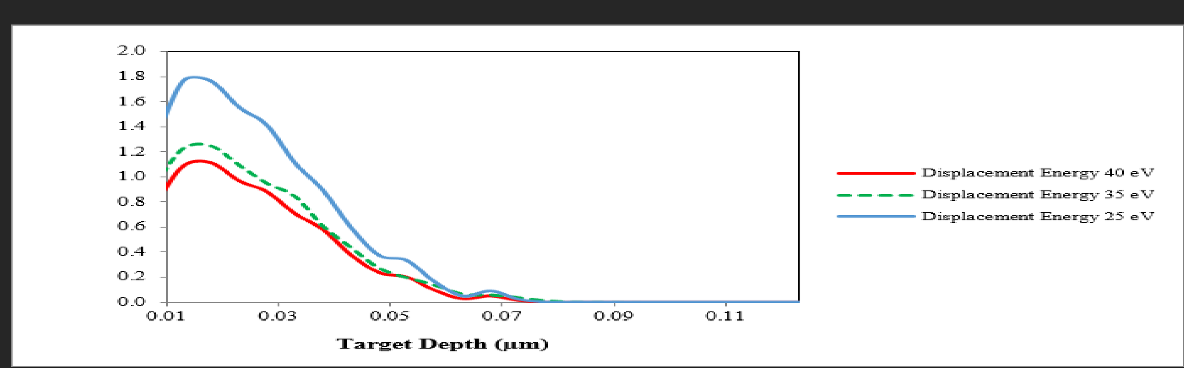


Fig.5. Fe ions 50KeV in Zr target layer (K-P)

Conclusion

Its frequently being mentioned that there is a recommendation on setting binding energy value in SRIM calculations to zero. We have investigated the impact of this parameter on the calculated damage results by using both the recommended (0 eV) and default (3 eV) values and both SRIM K-P and F-C calculations modes and also it was found change by using different energy displacements .