Forschungszentrum Karlsruhe
in der Helmholtz-Gemeinschaft

Calculation of displacement cross sections at intermediate and high energies of primary particles using results of molecular dynamics simulations

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Introduction

Available experimental data show the difference with predictions of the NRT model (*Norget, Robinson, Torrens*, 1975) implemented in NJOY, MCNPX, SPECTER etc)

The idea is to perform combined calculations using

- intranuclear cascade evaporation model (INC),
- binary collision approximation model (BCA)
- molecular dynamics simulations (MD).

The displacement cross-section is equal to

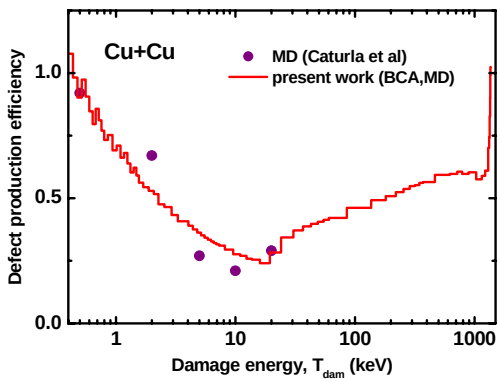
$$\sigma_d(E_p) = \sum_i \int_{E_d}^{T_i^{max}} \frac{d\sigma(E_p, T_i, Z_T, A_T, Z_i, A_i)}{dT_i} \nu(T_i) dT_i \quad ,$$

$d\sigma/dT_i$ is the recoil energy distribution,
$\nu(T_i)$ is the number of Frenkel pairs produced by PKA,
$\nu(T) = \eta(T) \cdot N_{NRT}(T)$,
N_{NRT} is the number of defects predicted by NRT,
$N_{NRT} = 0.8 \cdot T_{dam}/(2E_d)$, T_{dam} is the "damage energy"
$\eta(T)$ is the defect production efficiency.

Calculation of the number of defects produced under irradiation

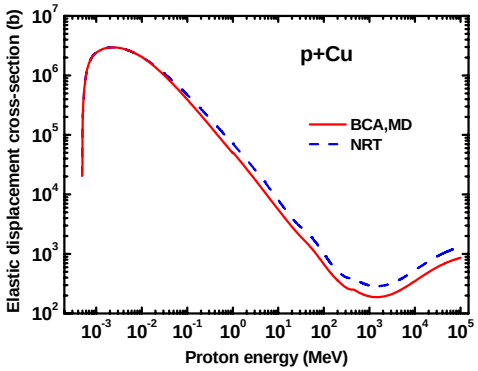
For an energetic ion moving in the material the simulation of the atomic collision is performed

- by the BCA model up to a certain "critical" energy of the ion, T_{crit},
- below T_{crit} the BCA calculation is stopped and the number of defects is evaluated according to results of the MD simulation.



Example of combined BCA-MD calculations. The critical energy for Cu-ion is equal to 28.3 keV. The maximal T_{dam} (NRT) energy corresponds to the primary energy of Cu-ions 5 GeV.

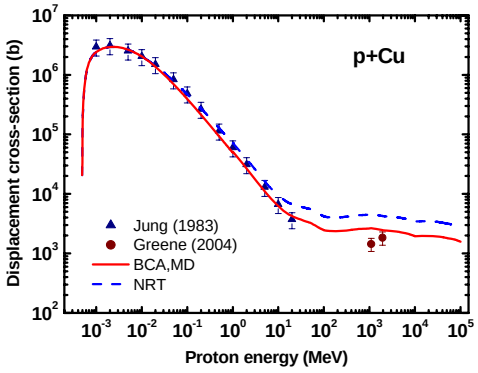
3. Calculation of displacement cross-sections for proton induced reactions



The elastic displacement cross-section for copper.

The displacement cross-section ($\sigma_{d,non}$) (b) for nonelastic interactions p+^{63}Cu at E_p= 150 MeV

Nuclear model	BCA-MD	NRT
Bertini/Dresner	1790	3060
Bertini/ABLA	1890	3230
ISABEL/Dresner	1730	2950
ISABEL/ABLA	1820	3110
CEM03	1780	3050
INCL4/Dresner	1920	3260
INCL4/ABLA	2010	3410
FLUKA/Dresner	2400	4050
FLUKA/ABLA	2510	4220
CASCADE	1740	3000
DISCA-C	2070	3500
Average value	1970±270	3350±430



The total displacement cross-section for copper

Conclusion

Displacement cross-sections obtained using the INC model, the BCA model, and results of MD simulations are in the better agreement with available experimental data than cross-sections calculated on the basis of the NRT model.