National Research Centre «Kurchatov Institute»

Radiation-induced diffusion of interstitial atoms under heavy ion irradiation

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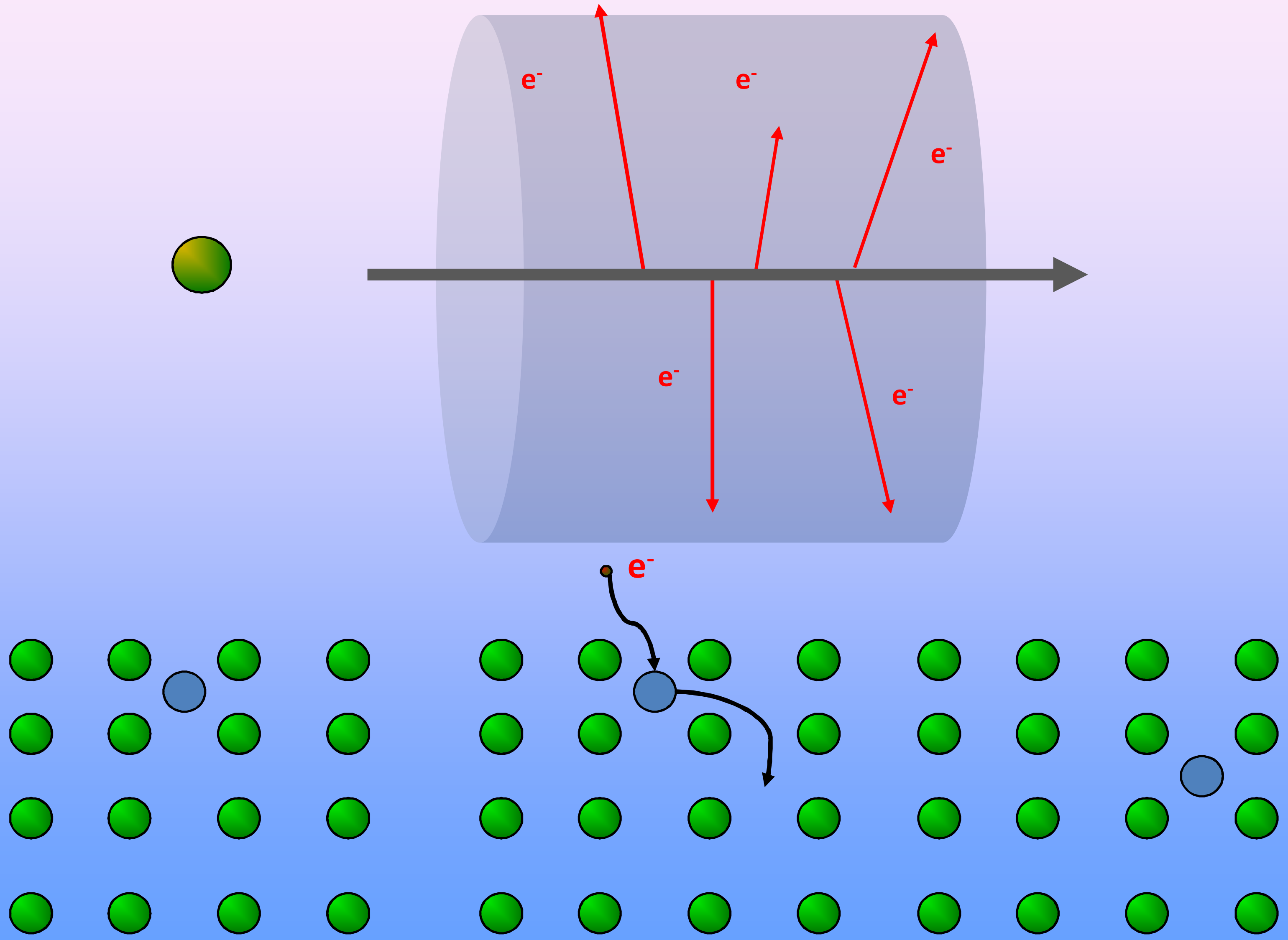
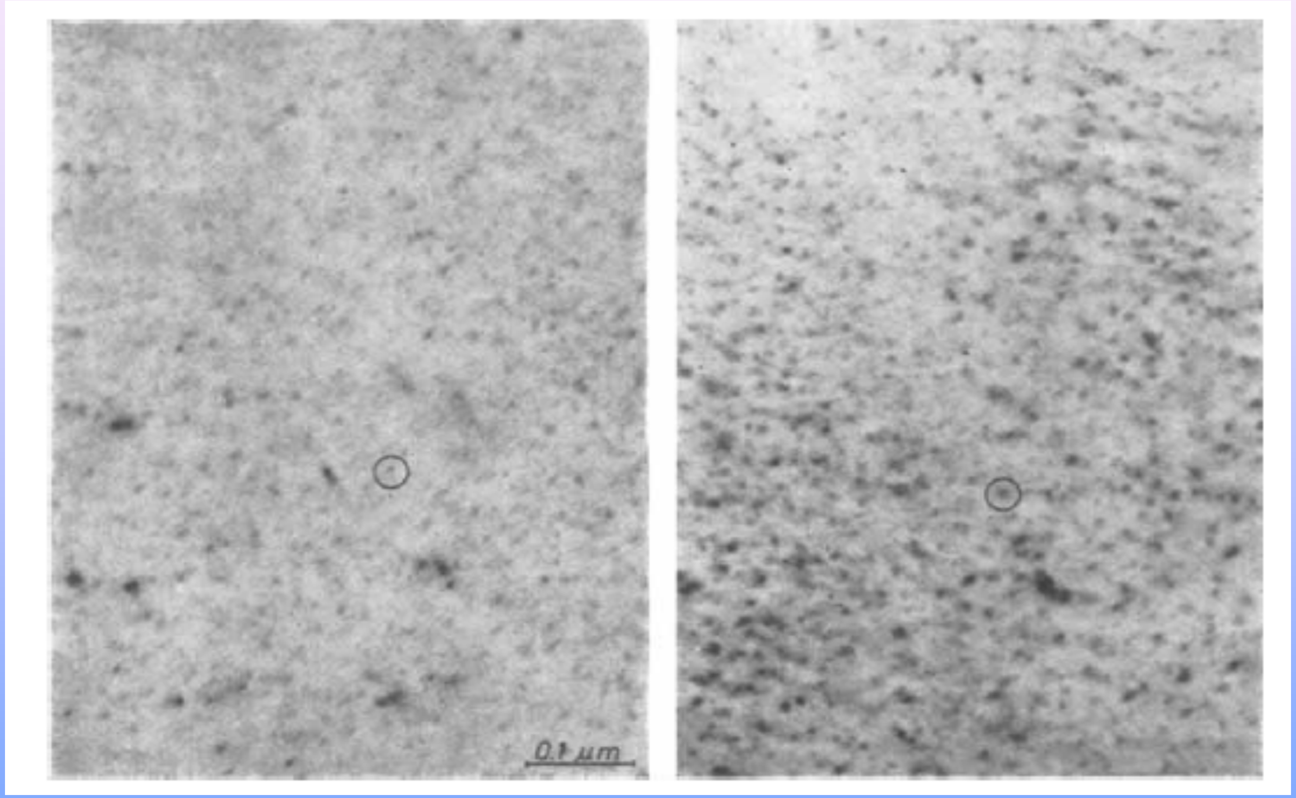
A scheme of radiation-induced diffusion process of interstitials due to heavy ion impact



ICTP-IAEA Workshop, Italy, 2011

Radiation-induced diffusion in HVEM experiments



Urban and Seeger, 1974

The equation describing the steady slowing-down of particles in a homogeneous nonabsorbing medium from a uniform source can be written as follows:

$$\Sigma(\varepsilon)\Phi(\varepsilon) = \int_0^\infty d\varepsilon' \Sigma(\varepsilon' \to \varepsilon)\Phi(\varepsilon') + S(\varepsilon)$$

$$\Phi(\varepsilon) = \frac{S(\varepsilon)}{\Sigma(\varepsilon)} + \frac{1}{\Delta(\varepsilon)\Sigma(\varepsilon)} \int_\varepsilon^{\varepsilon_0} S(\varepsilon')d\varepsilon'$$

Differential cross section for inelastic scattering of electrons on the atom has the form:

$$\Sigma(\varepsilon' \to \varepsilon) = \frac{\pi Z_2 e^4 n_0}{\varepsilon'} \frac{dT}{T^2}$$

The energy distribution of electrons produced by high energy particle:

$$S_1(\varepsilon) = \Phi_1 \frac{\pi n_0 Z_2 Z_1^2 e^4 M_1}{m E_1} \frac{1}{\varepsilon^2}$$

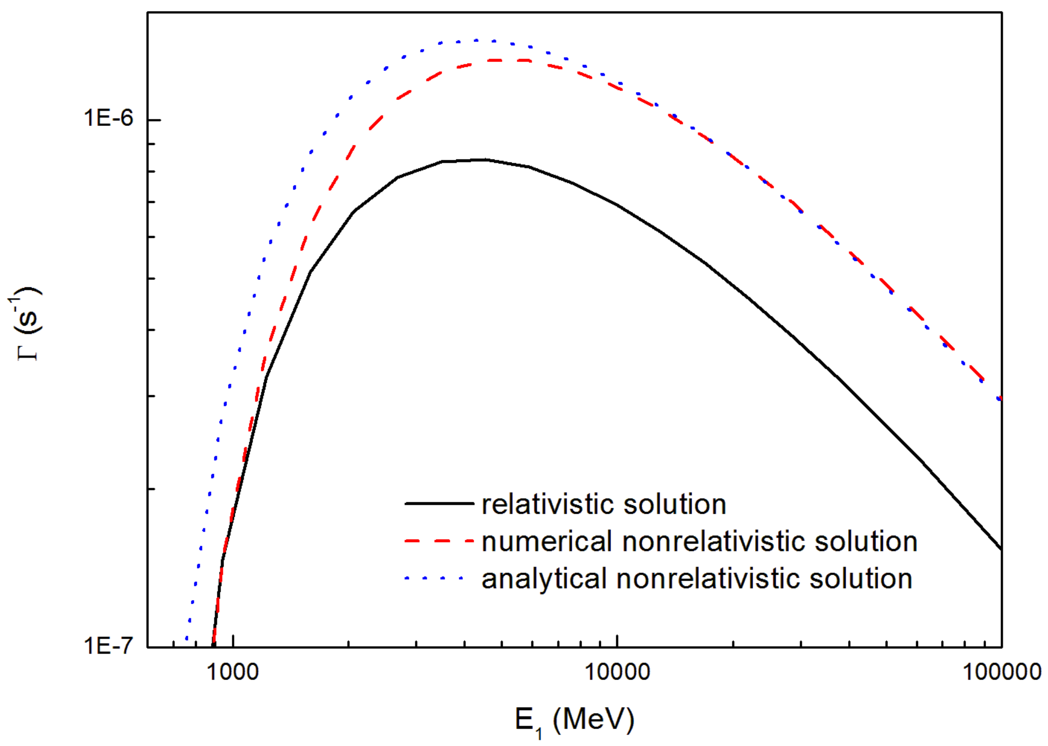
Collision frequency of slowing-down electrons accompanied by a knock-on of interstitial atoms can be found by the formula:

$$\gamma_a = \int_{\varepsilon_a}^{\varepsilon_m} d\varepsilon \Phi(\varepsilon) \sigma_{ei}(\varepsilon)$$

Collision frequency of slowing-down electrons accompanied by a knock-on of interstitial atoms can be found by the formula:

$$\gamma_a = \Phi_1 \frac{\pi e^4 Z_1^2 Z_2^2 I}{2\varepsilon_m \varepsilon_a^2} \left\{ \left(1 - \frac{\varepsilon_a}{\varepsilon_m}\right)^2 + \frac{2\varepsilon_a}{I} \left[\left(1 + \frac{\varepsilon_a}{\varepsilon_m}\right) \ln\left(\frac{\ln\left(\frac{\varepsilon_m}{I}\right)}{\ln\left(\frac{\varepsilon_a}{I}\right)} \right) - \left(1 - \frac{\varepsilon_a}{\varepsilon_m}\right) \left(\frac{1}{\ln\left(\frac{\varepsilon_m}{I}\right)} + \frac{1}{\ln\left(\frac{\varepsilon_a}{I}\right)} \right) \right] \right\}$$

Comparison of relativistic and nonrelativistic cases for collision frequencies delta-electrons. Analytical solution is also included



Inelastic scattering cross section of electrons for relativistic case

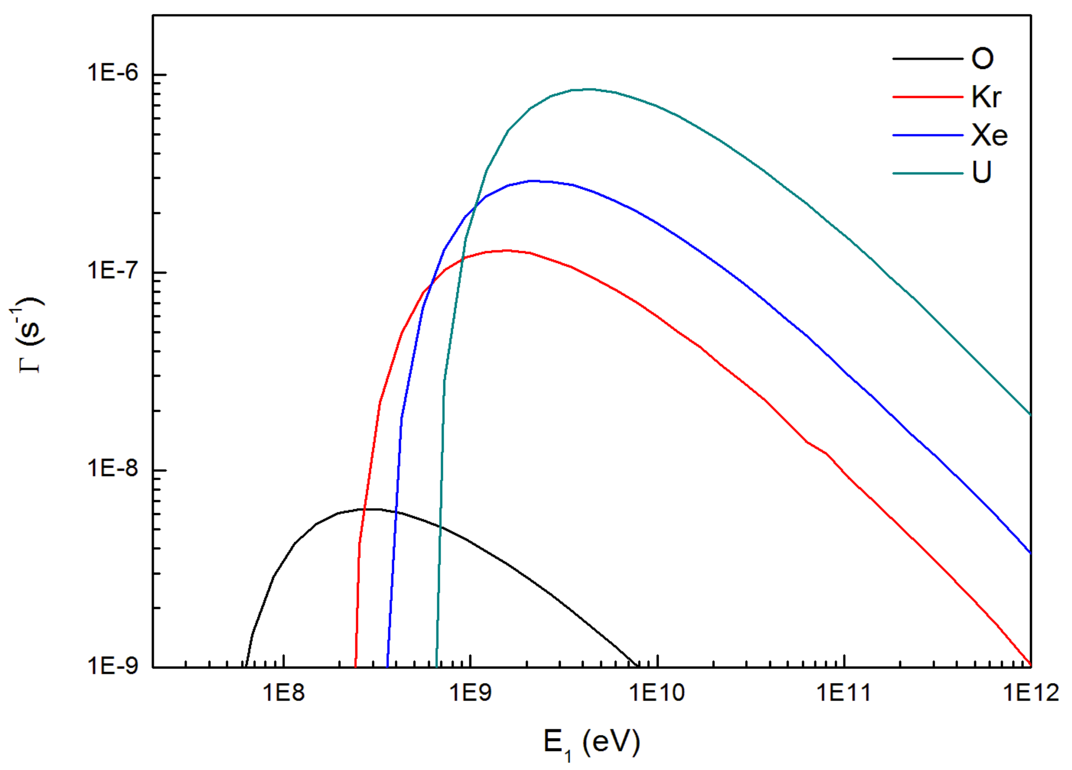
$$\frac{d\sigma}{dT} = \frac{2\pi e^4}{mv^2}\left[\frac{1}{T^2} + \frac{1}{(\varepsilon - T)^2} - \frac{1}{T(\varepsilon - T)} + \left(\frac{\gamma - 1}{\gamma}\right)^2 \left(\frac{1}{\varepsilon^2} + \frac{1}{T(\varepsilon - T)}\right)\right]$$

$$\gamma = 1 + E / mc^2$$

Elastic scattering cross section of electrons for relativistic case

$$\frac{d\sigma(E, E_e)}{dE} = \frac{4\pi a_0{}^2 Z_T{}^2 E_R{}^2}{m_e{}^2 c^4} \cdot \frac{1 - \beta^2}{\beta^4}\left[1 - \beta^2 \frac{E}{E_m} + \pi \frac{Z_T \beta}{137}\left\{\left(\frac{E}{E_m}\right)^{\frac{1}{2}} - \frac{E}{E_m}\right\}\right] \cdot \frac{E_m}{E^2}$$

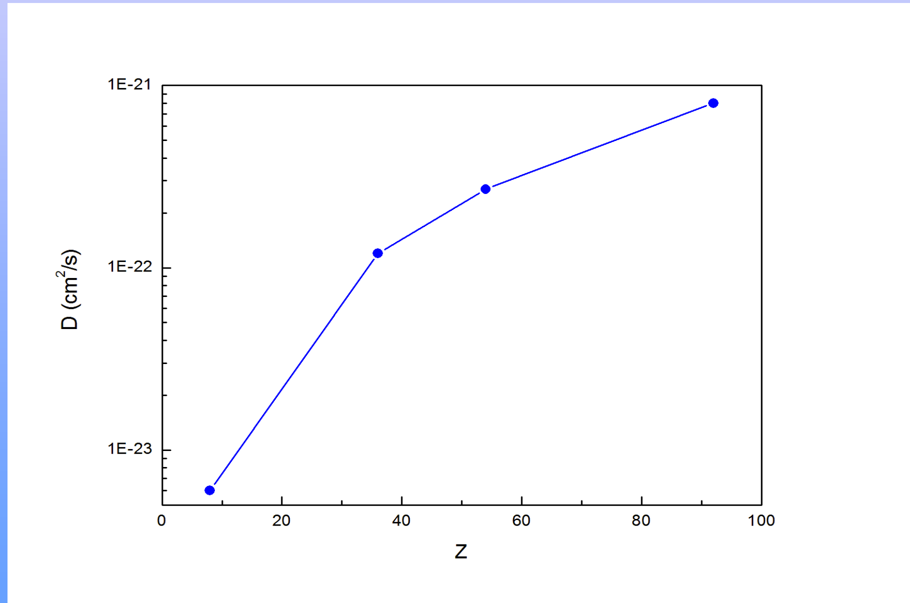
Collision frequency of δ-electrons with interstitials in iron calculated for heavy ion irradiation with energy higher than 1 MeV/nucl



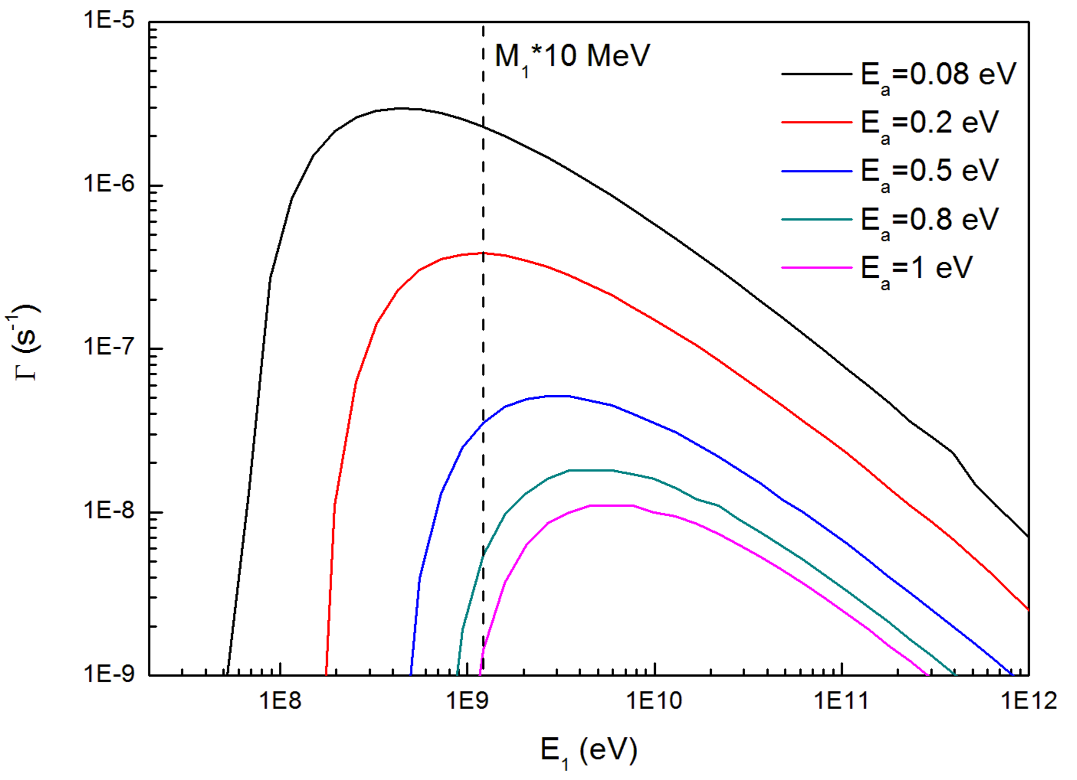
Radiation-induced diffusivity can be calculated using collision frequency and mean square displacement of interstitial atoms:

$$D = \frac{1}{6} < R^2 > \gamma$$

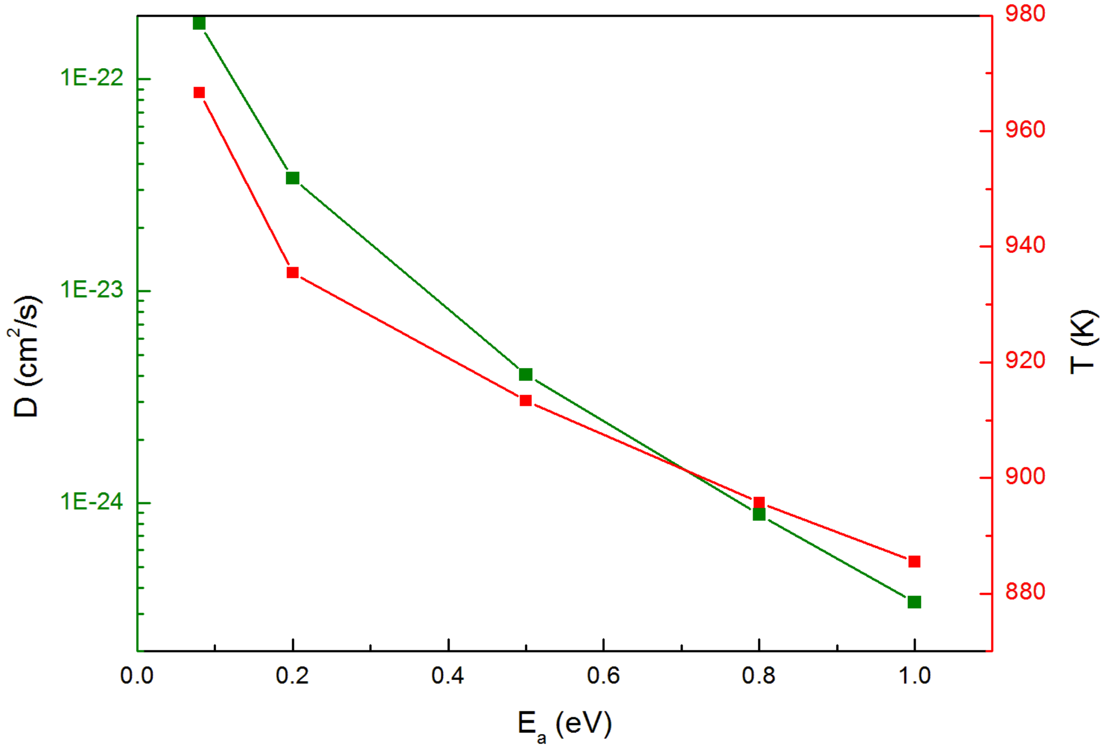
Maximum radiation-induced diffusivity of interstitials for irradiation with different atomic numbers for silicon



Collision frequency of δ-electrons with interstitials in silicon calculated for Xe ion irradiation with different activation energies. Flux value of 10^{10} ions/(cm^2*c) is used in this calculations



Diffusivity of SIA in silicon and effective temperature increase as a functions of activation energy



Summary

On the basis of the Boltzmann equation a model is proposed for calculating the radiation-induced diffusivity due to secondary processes (ionization)

The data obtained suggest that the ionization process by heavy ions with energies higher than 100 MeV/nucl. have no direct effect on the process of radiation-induced diffusion as diffusivity curve has a maximum corresponding to the energy range of 5-10 Mev/nucl. for heavy ion irradiation.

The influence of relativistic and exchange effects in both elastic and inelastic interaction of electrons is taken into account. It's shown that the inclusion of these effects reduce the of radiation-induced diffusivity of approximately one order of magnitude. The dependence of the diffusion coefficient of the activation energy of interstitial atoms in silicon and the energy of the heavy ion at a fixed flux.

At a fixed flux of heavy ion irradiation, diffusivity is slowly increasing for light target materials with small atomic numbers. The actual impact of radiation-induced diffusion is highly depends of actual mobility of interstitials and its mean square displacement. Thus one may conclude that radiation induced diffusion plays important role in semiconductor materials and targets with low atomic numbers such as graphite.