Non-ionizing energy loss calculations for modeling electron-induced degradation of Cu(In, Ga)Se_2 thin-film solar cells*

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The lowest energies which make Cu, In, Ga, and Se atoms composing Cu(In, Ga)Se_2 (CIGS) material displaced from their lattice sites are evaluated, respectively. The non-ionizing energy loss (NIEL) for electron in CIGS material is calculated analytically using the Mott differential cross section. The relation of the introduction rate (k) of the recombination centers to NIEL is modified, then the values of k at different electron energies are calculated. Degradation modeling of CIGS thin-film solar cells irradiated with various-energy electrons is performed according to the characterization of solar cells and the recombination centers. The validity of the modeling approach is verified by comparison with the experimental data.

Keywords: Cu(In, Ga)Se_2 solar cells, non-ionizing energy loss, electron irradiation

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1. Introduction

Cu(In, Ga)Se_2 (CIGS) thin-film solar cells have been considered as one of the most promising candidates for space application, having high efficiency exceeding 21%, lightweight, flexible and high radiation tolerance.[1,2] Exposure to the space radiation environment degrades the performance of solar cells, even causing the failure of the space mission.[3,4] Consequently, it is extremely important to predict the degradation of solar cells induced by electron and proton.

Previous studies on the degradation of CIGS solar cells were based on ground test and space flight experiment.[5,6] Essentially, the degradation of solar cells induced by electron irradiation is directly related to the concentrations of the recombination centers, which can be detected and identified among all the defects by photoluminescence.[7,8] In order to improve the radiation resistance of solar cells, the study on injection-enhanced annealing of electron irradiation-induced defects was carried out by temperature-dependent photoluminescence.[9,10] However, the experimental characterization is time consuming and can be very expensive. As a result, a modeling method was proposed to predict the degradation of solar cells based on classical semiconductor equations.[11] The key of this method is the determination of the introduction rates (k) of the recombination centers, but the values of k at several specific electron energies are merely provided for CIGS solar cells. In order to predict the degradation of CIGS solar cells systematically, the values of k need to be given for various-energy electrons. This purpose can be achieved by obtaining non-ionizing energy loss (NIEL), which is analogous to the linear energy transfer or stopping power for ionization events.[11,12]

In this paper, firstly, the electron-induced NIEL in the CIGS material is computed by an analytic method. Secondly, the values of k for different energy electrons are confirmed by NIEL. Finally, the degradation of CIGS solar cells irradiated with various-energy electrons is predicted by a theoretical calculation according to the characterization of solar cells and the recombination centers.

2. Principle of modeling

In this work, CIGS solar cells which have an average bandgap energy of around 1.16 eV (corresponding to Ga/(Ga + In) $\approx$ 0.24) are chosen as the research object. Figure 1(a) shows the schematic cross-section of a typical CIGS solar cell which consists of an antireflection layer, transparent conducting oxide (TCO), a CdS buffer layer, a CIGS absorber layer, an Mo layer as a back contact and substrate.[13] Generally, the CIGS solar cells are considered as a one-side abrupt heterojunction, for which the depletion region is virtually located in the lightly doped CIGS layer (see Fig. 1(b)) and the photoelectric conversion almost takes place in this layer.[14]

Therefore, the short circuit current density $J_{SC}(\lambda)$ at a given wavelength is the sum of the photocurrent density generated in the depletion region (DR) $J_{DR}(\lambda)$ and in the quasi-neutral region (QNR) $J_{QNR}(\lambda)$ as

$$J_{SC}(\lambda) = J_{DR}(\lambda) + J_{QNR}(\lambda). \quad (1)$$

The total short circuit current density J_{SC} when the sunlight with a spectral distribution $F_0(\lambda)$ is incident on the solar

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cells is found by integrating Eq. (1) as

$$J_{\rm SC} = q\int_{\lambda_1}^{\lambda_2}[J_{\rm DR}(\lambda)+J_{\rm QNR}(\lambda)]{\rm d}\lambda, \tag{2}$$

where q is the electron charge, λ_1 is the lowest wavelength for which $F_0(\lambda)$ is non-negligible, and λ_2 corresponds to the limit of absorption.

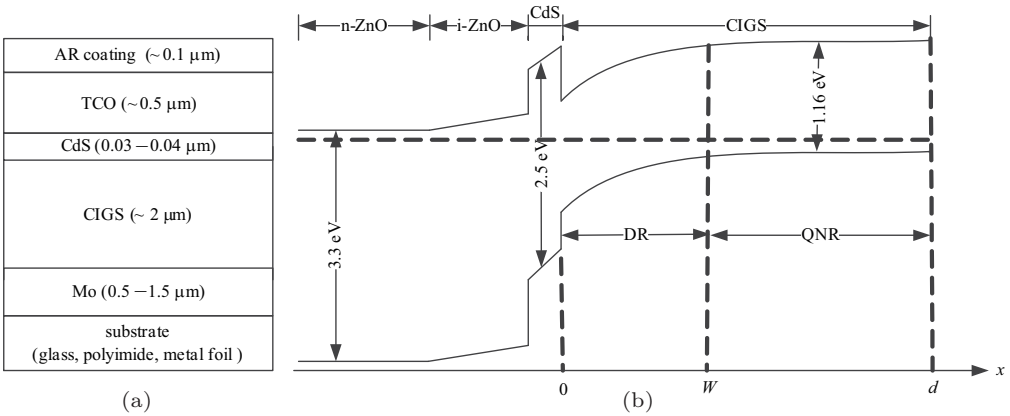


Fig. 1. (a) Typical structure for CIGS solar cells. (b) Schematic band diagram of CIGS solar cells under zero-bias voltage condition.

Taking into account the surface recombination at the CdS/CIGS interface, under zero-bias, $J_{\rm DR}(\lambda)$ can be written as[13,15]

$$J_{\rm DR}(\lambda) = qF_0(1-R)\left[\frac{1+(S/D_{\rm p})[\alpha+(2/W)qV_{\rm bi}/k_{\rm B}T]^{-1}}{1+(S/D_{\rm p})[(2/W)qV_{\rm bi}/k_{\rm B}T]^{-1}} - \exp(-\alpha W)\right], \tag{3}$$

where R is the reflectivity, S is the velocity of recombination at the CdS/CIGS interface, $D_{\rm p}$ is the diffusion coefficient of holes, α is the absorption coefficient of CIGS material, W is the width of the depletion region, $V_{\rm bi}$ is the built-in potential, $k_{\rm B}$ is Boltzman constant, and T is the temperature.

By considering the recombination at the back surface of the CIGS layer, $J_{\rm QNR}(\lambda)$ is given by[15]

$$J_{\rm QNR}(\lambda) = \frac{qF_0(1-R)\alpha L_{\rm n}}{\alpha^2 L_{\rm n}^2-1}\exp(-\alpha W) \times\left[\alpha L_{\rm n}-\frac{(S_{\rm b}L_{\rm n}/D_{\rm n})[\cosh((d-W)/L_{\rm n})-\exp(-\alpha(d-W))]+\sinh((d-W)/L_{\rm n})+\alpha L_{\rm n}\exp(-\alpha(d-W))}{(S_{\rm b}L_{\rm n}/D_{\rm n})\sinh((d-W)/L_{\rm n})+\cosh((d-W)/L_{\rm n})}\right], \tag{4}$$

where $S_{\rm b}$ is the velocity of recombination at the back surface of the CIGS layer, d is the thickness of the CIGS absorber layer, $L_{\rm n}=\sqrt{D_{\rm n}\tau_{\rm n}}$ is the electron diffusion length, $D_{\rm n}$ is the diffusion coefficient of electrons, and $\tau_{\rm n}$ is the minority carrier lifetime.

The basic solar cells equation incorporating recombination losses is expressed as

$$J = J_{\rm SC}-J_{01}\left[\exp\left(\frac{qV}{k_{\rm B}T}\right)-1\right]+J_{02}\left[\exp\left(\frac{qV}{2k_{\rm B}T}\right)-1\right], \tag{5}$$

where J and V are the current density and voltage, respectively, J_{01} and J_{02} are given by the following expressions:

$$J_{01} = \frac{qn_{\rm i}^2}{N_{\rm A}}\sqrt{\frac{D_{\rm n}}{\tau_{\rm n}}}, \tag{6}$$

$$J_{02} = \frac{qWn_{\rm i}}{2\tau_{\rm n}}. \tag{7}$$

In the above expressions, $n_{\rm i}$ is the intrinsic carrier concentration and $N_{\rm A}$ is the doping concentration.

In the condition of open circuit, $V = V_{\rm OC}$ (open circuit voltage), $J = 0$. According to Eq. (5), the relation of $V_{\rm OC}$ to $J_{\rm SC}$ can be derived as follows:

$$V_{\rm OC} = \frac{2k_{\rm B}T}{q}\ln\left(\frac{-J_{02}+\sqrt{J_{02}^2+4J_{01}(J_{\rm SC}+J_{01}+J_{02})}}{2J_{01}}\right). \tag{8}$$

Recombination centers cause the performance degradation of solar cells by reducing the minority carrier lifetime[15]

$$\frac{1}{\tau_{\rm n}} = \frac{1}{\tau_0}+k\sigma\nu\varphi, \tag{9}$$

where τ_0 is the minority carrier lifetime before irradiation, σ is the minority carrier trapping cross section, ν is the thermal velocity of carriers, and φ is the irradiation fluence.

3. Calculation of NIEL

The NIEL is a quantity that describes the rate of energy loss due to atomic displacements when particles traverse a certain material. Atomic displacements can be produced only if

the maximum transferred energy (T_m) is more than the displacement energy (T_d). The T_d was calculated as being 9.8 eV, 15.6 eV, 12.4 eV, and 28.5 eV for Cu, In, Ga, and Se atoms in CIGS material, respectively.[16] The T_m can be given by[17]

$$T_m = \frac{2E(E+1.022)}{M_0c^2A}, \tag{10}$$

where E is the incoming electron energy in MeV, A is the atomic mass of target atoms, and M_0c^2 is the equivalent energy for 1 AMU, i.e., 931.5 MeV.

Figure 2 shows the variation of T_m versus E for Cu, In, Ga, and Se atoms in CIGS material, respectively. It is noted that T_m increases with the increase of E. According to T_d for Cu, In, Ga, and Se atoms, electron energy can be divided into five regions: (i) $E \leq\sim 0.23$ MeV, no vacancies are produced, (ii) ~ 0.23 MeV$< E \leq\sim 0.30$ MeV, only Cu vacancies (V_{Cu}) are probably produced, (iii) ~ 0.30 MeV$< E \leq\sim 0.53$ MeV, Cu and Ga vacancies (V_{Cu} and V_{Ga}) are probably produced, (iv) ~ 0.53 MeV$< E \leq\sim 0.63$ MeV, Cu, In and Ga vacancies (V_{Cu}, V_{In} and V_{Ga}) are probably produced, (v) $E >\sim 0.63$ MeV, Cu, In, Ga, and Se vacancies (V_{Cu}, V_{In}, V_{Ga}, and V_{Se}) are probably produced.

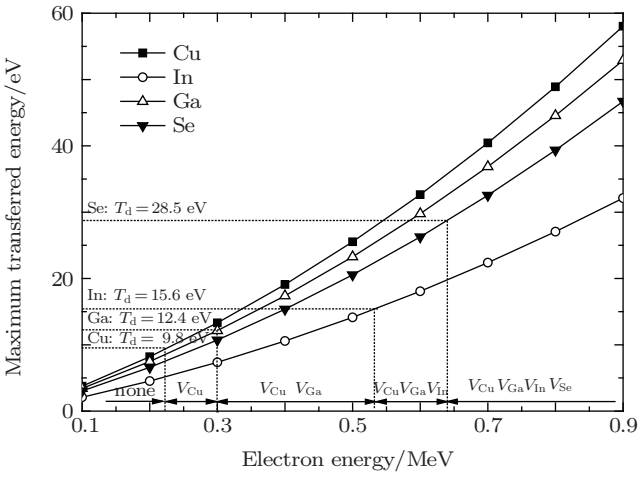


Fig. 2. Maximum transferred energy of Cu, In, Ga, Se atoms composing CIGS material.

Figure 3 shows the electron NIEL for Cu, In, Ga, Se atoms and $CuIn_{0.76}Ga_{0.24}Se_2$ compound. The electron NIEL is calculated by an analytic method using the Mott differential cross section, then NIEL for the $CuIn_xGa_{1-x}Se_2$ compound can be estimated by the ratio of atoms in this material as[17]

$$\mathrm{NIEL}_{CuIn_xGa_{1-x}Se_2} = \frac{\mathrm{NIEL}_{Cu}A_{Cu} + \mathrm{NIEL}_{In}A_{In}x + \mathrm{NIEL}_{Ga}A_{Ga}(1-x) + 2\mathrm{NIEL}_{Se}A_{Se}}{A_{Cu} + A_{In}x + A_{Ga}(1-x) + 2A_{Se}}. \tag{11}$$

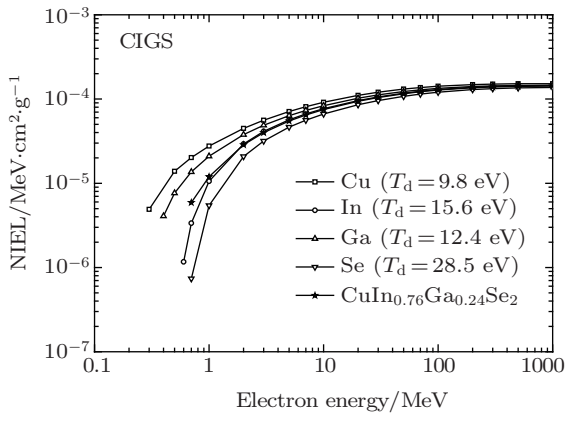


Fig. 3. NIEL of Cu, In, Ga, Se atoms and $CuIn_{0.76}Ga_{0.24}Se_2$ compound.

4. Derivation of the introduction rate

The correlation between the introduction rate (k) and NIEL can be written as[11]

$$k = \beta \mathrm{NIEL}, \tag{12}$$

where β is a constant.

For 1-MeV electron, $k = 0.02$ cm^{-1}[18] and NIEL $= 1.2 \times 10^{-5}$ MeV $\cdot$ cm^2 $\cdot$ g^{-1}. Hence, $\beta = 1.67 \times 10^3$ g$\cdot$MeV$^{-1}\cdot$cm^{-3}. For 3-MeV electron, NIEL $= 3.99 \times 10^{-5}$ MeV$\cdot$cm$^2\cdot$g^{-1}. According to Eq. (12), $k = 0.07$ cm^{-1} is obviously different from the value (0.2 cm^{-1}) in Ref. [18]. Therefore, by analogy to the relation of the displacement damage dose to electron NIEL,[19] k is modified as follows:

$$k = \beta \mathrm{NIEL}(E)\left(\frac{\mathrm{NIEL}(E)}{\mathrm{NIEL}(1\ \mathrm{MeV})}\right)^{n-1}, \tag{13}$$

where n is a constant and $1 < n < 2$.

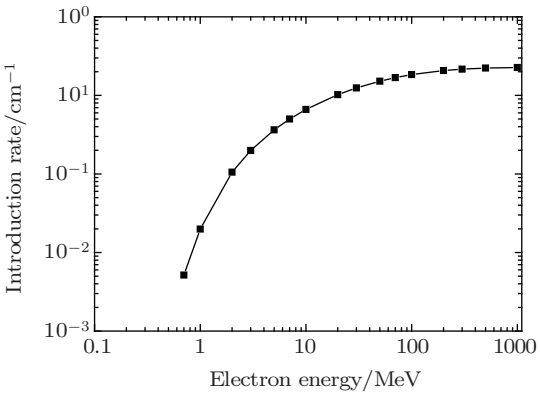


Fig. 4. The introduction rate of recombination centers for different energy electron irradiation.

Substituting the values of k and NIEL for 1-MeV and 3-MeV electron in Eq. (13), we obtain $n = 1.91$ and $\beta = 1.67 \times 10^3$ g$\cdot$MeV$^{-1}\cdot$cm^{-3}. Therefore, using Eq. (13), more

values of k at different electron energy can be calculated. Figure 4 shows the dependence of k versus electron energy. As seen in Fig. 4, the rate k increases with electron energy increasing, but the rate of increase gradually decreases.

5. Degradation of CIGS solar cells

In order to predict the degradation of CIGS solar cells, the physical parameters of solar cells used in calculations are listed in Table 1.

Table 1. The physical parameters of CIGS solar cells.

Symbol	Parameter	Value
μ_n	electron mobility	20 $cm^2 \cdot V^{-1} \cdot s^{-1}$ [a]
μ_p	hole mobility	30 $cm^2 \cdot V^{-1} \cdot s^{-1}$ [a]
R	reflectivity	Ref. [13]
α	absorption coefficient	Ref. [13]
N_C	effective density of states in the conduction band	2.2×10^{18} cm^{-3} [b]
N_V	effective density of states in the valence band	1.8×10^{19} cm^{-3} [b]
N_A	doping concentration	2×10^{16} cm^{-3}
τ_0	minority carrier lifetime	100 ns
σ	minority carrier trapping cross section	3×10^{-16} cm^2
v	thermal velocity of carriers	4×10^7 cm/s

[a]Ref. [13], [b]Ref. [20].

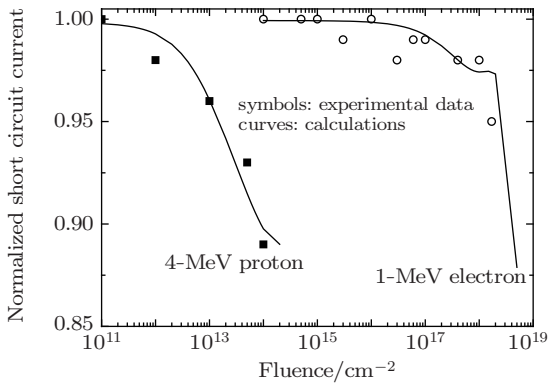


Fig. 5. Normalized short circuit current of CIGS solar cells irradiated with 1-MeV electron and 4-MeV proton. Curves are the results of calculations, and symbols are experimental data taken from Ref. [18].

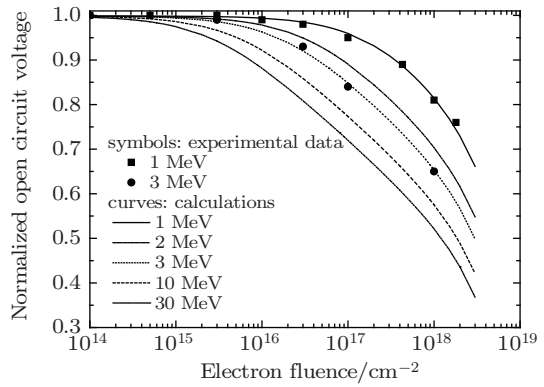


Fig. 6. Normalized open circuit voltage of CIGS solar cells irradiated with various-energy electrons. Curves are the results of calculations, and symbols are experimental data taken from Ref. [18].

Figure 5 shows the degradation of normalized short circuit current for CIGS solar cells under 1-MeV electron and 4-MeV proton ($k = 1000$ cm^{-1} [18]) irradiation. Figure 6 shows the degradation of open circuit voltage for CIGS solar cells under various-energy electron irradiation, and also presents the experimental data taken from Ref. [18] for 1-MeV and 3-MeV electrons. As shown in Figs. 5 and 6, the degradation curves obtained from calculations show good agreement with experimental data. This ensures the validity of the modelling method and the accuracy of calculations.

6. Conclusion

When electron energy $E \leq \sim 0.23$ MeV, no vacancies are produced and the performance of CIGS solar cells will not degrade. Electron NIEL for CIGS material is calculated analytically. The relation of k to NIEL is modified, and the values of k for various-energy electrons are given. The degradation of CIGS solar cells under various-energy electron irradiation is predicted by a theoretical calculation. Accuracy of prediction can be ensured by the fact that the degradation curves obtained from the theoretical calculation are in good agreement with the experimental data.

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