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Multi-scale modelling of iron impurity in photovoltaic devices

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Iron is arguably the most important detrimental contamination in lower grade silicon, which is a problem in photovoltaic as interstitial iron (Fei) is understood to be an active recombination centre, lowering device efficiency. In this work, First-principles quantum-chemical simulations are combined with TCAD device modelling to examine the silicon properties with iron impurity, as an attempt to balance interoperation of the disadvantageous properties of these impurities on the performance of solar cells as function of iron concentration. The results show that Fe-impurity has reduced the hole density slightly with increasing iron concentration from 10^8 to 10^{16} cm^{-3}, whereas, the electron density is affected significantly with increasing the impurity concentration. In contrast, carrier mobilites are almost constant at low iron concentration, however, it is found that they are decreasing when iron concentration exceeds 10^{14} cm^{-3}. Moreover, it is found that the recombination rate is increasing due to the increase in the impurtiy concentration. Finally, it is noticed from these figures that short-circuit current density (Jsc) has been reduced by around 47% with increasing the Fe concentration from 10^8 to 10^{16} cm^{-3}. On the other hand, the open-circuit voltage (Voc) is reduced by around 27% within the same range of impurity concentration. These changes in the Jsc and Voc have led to degradation in the total conversion efficiency from 16% to 6%. Furthermore, the role of iron impurities play in iron-precipitation and segregation to, for example, extended defects, is of key interest for the solar cell performance.

Biography

Oras A Al-Ani is currently studying towards the PhD degree within the Emerging Technologies and Material (ETM) group, School of Electrical and Electronics Engineering, Newcastle University, UK. Her research focuses on computational and theoretical analysis of the point and extended defects in multicrystalline silicon and their impact on photovoltaic devices. She serves as research student representative in EEE School, the IEEE student branch committee member as well as member of IET, IEEE and Al-Kindi Society for Engineers; and awarded several awards for the best paper and presentation. She is currently acting as the Student Ambassador for Materials Congress 2016.

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