Iron pyrite (cubic FeS$_2$) is a candidate for photovoltaic device material because of its strong light absorption ($\alpha > 10^5$ cm$^{-1}$ for hv > 1.3 eV), earth-abundance and low cost [1,2]. Moreover bulk n-type iron pyrite single crystal has high majority carrier mobility (> 300 cm$^2$V$^{-1}$s$^{-1}$) and long minority carrier diffusion length (L = 0.1 – 1 μm) [1,3]. Therefore, iron pyrite offer a great opportunity for developing sustainable and inexpensive photovoltaic device [4]. Nevertheless, it has an especially short-circuit current ($J_{SC}$) of 42 mA/cm$^2$, good quantum efficiency (Maximum 90% at 380 – 1330 nm), a low open-circuit voltage ($V_{OC}$) of below 0.2 V and a moderate fill factor (FF) of 50% that limits conversion efficiency to 2.8% [1]. This reported cell is photoelectrochemical (PEC) solar cell which is fabricated with n-type iron pyrite crystal grown by chemical vapor transport method and iodine/iodide aqueous electrolyte [1]. Recently FeS$_2$ thin film was prepared with various method and applied to photovoltaic device, however these cells did not record a conversion efficiency. Its poor characteristics are possibly an effect by an inversion layer at the surface of iron pyrite and deep donor level in bulk [5,6]. We modeled the FeS$_2$ solar cell including the density of state and calculated the solar cell performance to understand the effect of high deep donor level and inversion layer to iron pyrite photovoltaic device and realize a plan for realization of FeS$_2$ solar cell. In this study, 2D ATLAS device simulator (Silvaco Inc.) was utilized to design FeS$_2$ solar cell on the basis of the drift-diffusion transport model.

FeS$_2$ was n-type semiconductor, so Cu$_2$O was utilized as p-type semiconductor having wide band gap to model p-Cu$_2$O/n-FeS$_2$ hetero junction solar cell. Figure 1 shows the I-V characteristics of ITO/Cu$_2$O/FeS$_2$/Al device under both dark and illumination condition. The conversion efficiency of ITO/Cu$_2$O/FeS$_2$/Al device including FeS$_2$ inversion layer was 0.52%. On the other hand, the cell without FeS$_2$ inversion layer increased conversion efficiency to 1.20%. Removing FeS$_2$ inversion layer increased conversion efficiency, however the effect was not significant. This causes a high defect density of FeS$_2$ bulk layer and short lifetime. Previous research reported that the defect density of FeS$_2$ bulk layer was $6.3 \times 10^{18}$ cm$^{-3}$ and lifetime was 270 ps [5,6]. Here we calculated the effect of defect density and lifetime on solar cell characteristic. Figure 2 shows the calculation result. The conversion efficiency was increased by improvement of defect density and lifetime. The efficiency reached the theoretical limit conversion efficiency of FeS$_2$ (16%) owing to the improvement of defect density and lifetime as well as applying anti-reflecting coat and optimizing film thickness of ITO and Cu$_2$O which decrease reflectance, leading to increasing $J_{SC}$.