Two dimensional nanostructures of transitional metal dichalcogenide semiconductor (TMDC) particularly MoS$_2$ binary compound is gaining wide attention due to its versatile electronic and optical properties. In this study, the influence of Mo microstructural properties on the formation of MoS$_2$ thin film through sulfurization process in investigated. Crystallographic properties of Mo thin film especially the degree of preferred orientation that alters the planar packing density is tailored through vacuum thermal annealing. Mo thin film, which possesses higher degree of (211) crystal orientation, exhibits pronounced formation of MoS$_2$ thin film compared to Mo thin film that consists of predominantly (110) crystal orientation. Planar packing density of Mo thin films with different crystal orientation is different and this is found to play a crucial role on the sulphur diffusion mechanism that ultimately influences the formation of MoS$_2$ (See Fig. 2). Hence, by controlling the Mo microstructural properties, the formation of MoS$_2$ layer and the resulting properties can be controlled. The implications of these findings are correlated to Cu$_2$ZnSnS$_4$ (CZTS) thin film solar cells whereby MoS$_2$ forms spontaneously through sulphur in-diffusion process from the CZTS absorber layer to the Mo back contact.

Figure 2: Interplay between planar packing density and Mo surface area