Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Efficiency enhancement due to self-organization of nano-structures in Cd(S, Te) solar cell material KAZUNORI SATO, Osaka University, PRESTO-JST, HIROSHI KATAYAMA-YOSHIDA, Osaka University — CdTe is one of the most important solar cell materials. Its energy gap is 1.44 eV, which is ideal for solar cell application. So far, conversion efficiency of 18.3 percent has been realized, but it is lower than the Shockley-Queisser limit. In this paper, we propose computational materials design for enhancing conversion efficiency by using self-organization in Cd(Te, S) alloy semiconductor. Firstly, we performed cluster expansion of total energy of the Cd(Te, S) system and simulated self-organization of nano-structures in Cd(Te, S) by using Monte Carlo method. It is found that layered structure becomes stable by applying strain during the crystal growth. The electronic structure of the self-organized layered structure was calculated by using the hybrid method (HSE06) implemented in the VASP code to derive optical absorption coefficient. By using the calculated absorption coefficient the efficiency limit was derived based on the Shockley-Queisser theory. It is shown that the efficiency limit does not change so much due to the nano-structure formation. However, our calculation shows spatial separation between photo-generated electrons and holes. This might enhance the efficiency due to the suppression of recombination.

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Date submitted: 14 Nov 2013 Electronic form version 1.4