Parallel Hybrid Simulation of CIGS Solar Cell Thin Film Deposition with the Co-Evaporation Method

C.-C. Su[1], K.-C. Tseng[2], Y.-S. Chen[2], J.-S. Wu[1*]

[1]Department of Mechanical Engineering, National Chiao-Tung University, Hsinchu 30050, Taiwan
[2]National Space Organization, National Applied Research Laboratories, Hsinchu 30078, Taiwan
*E-mail: chongsin@faculty.nctu.edu.tw

Introduction

The Copper Indium Gallium Selenide (CIGS) thin-film-based solar cell has attracted great attention recently in the energy related industry since it has higher efficiency (up to 20.5% for lab-scale cell), lower cost, and longer stability than the silicon-based solar cell. It will have great potential to the energy market if the in-line process of the CIGS deposition process could be achievable. However, the experimental test is still limited to the laboratory scale because the process is not easy to scale up to a larger area because of cost and technical reasons. Thus, simulations could be very helpful in designing the processing equipment, understanding these complicated deposition processes and operating conditions at very low cost and reduced time. In the current study, a hybrid simulation by combining the continuum and kinetic methods is presented and demonstrated for a typical co-evaporation method for CIG deposition onto glass surface.

Parallel Hybrid Numerical Simulation

Continuum N-S Equation Solver: UNIC-UNS Code

In modeling the surface-temperature distribution of melted metal, we have applied a CFD code named UNIC-UNS, which has been developed by Dr. Chen and his co-workers since 1995 [1]. It has several important features as summarized as follows: (1) cell-centered finite-volume method with a hybrid 2D/3D unstructured-grid topology, (2) a pressure-based method, which allows accurate simulation of the flows at all speeds, (3) automatic slip velocity and temperature jump boundary conditions near solid wall, (4) standard or extended k-e turbulence model, (5) two-phase model, (5) radiation transfer model, (6) conjugate heat transfer model, (7) chemical reactive flow model and (7) parallel computing using MPI library. This code is used to simulate the heat conduction of the heating evaporation sources.

DSMC Method: PDSC Code

In the current study, we have employed the previously developed Parallel DSMC Code (PDSC), which has been developed by Prof. Wu' group at NCTU since 2000 [2], for simulating the metal vapor transport from the melted surface to the glass. Several important features of PDSC were summarized as follows: (1)a spatially variable time step scheme to reduce the runtime to reach steady state (2) conservative weighting scheme for treating mixture with trace species, (3) pressure boundary treatment for internal flow simulations, (4) a gas phase chemistry model for simulating air chemical reactions in hypersonic flows and (5) parallel computing using dynamic domain decomposition, and a gas phase chemistry model for simulating chemical reactions in hypersonic air flows.

Hybrid Simulation Method

Figure 1 shows the proposed hybrid simulation procedure. We have first applied the UNIC-UNS code in calculating the surface temperature distribution of the melted metal and then it is imported into the PDSC code for evaluating the vapor pressure near the melted surface for DSMC simulation. Deposition flux distribution on the glass and flow properties in the chamber are then collected as the flow reaches steady state.

Figure 2 shows the sketch of an example CIGS film deposition process [3]. The three sources of copper, gallian and indium are heated by power leads. The selenium is provided as carrier gas that can be neglected in this simulation.

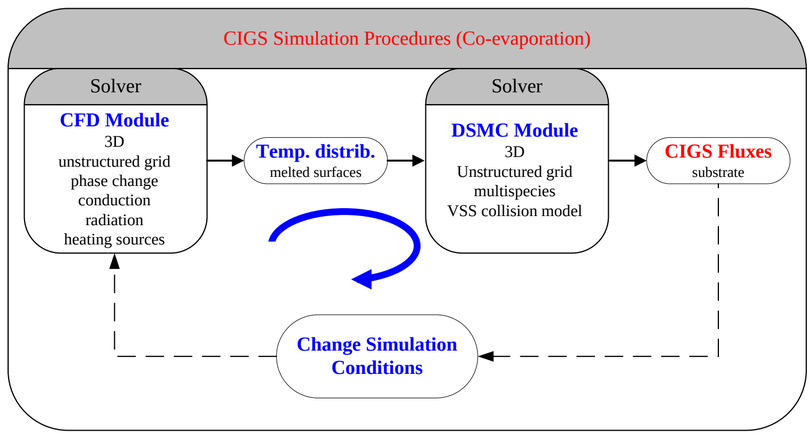

Figure 1: Proposed hybrid NS-DSMC simulation procedure.

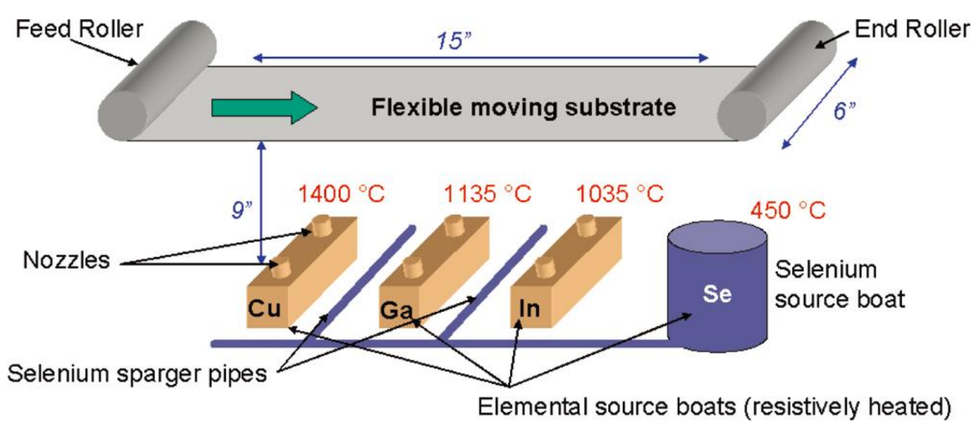

Figure 2: Sketch of the CIGS film deposition process using co-evaporation method [3].

Results and Discussion

The computational mesh and the temperature distribution of the three-dimensional copper source are shown in Figure 3. Two parallel power leads are embedded below the copper ingot, therefore you can see the temperature distribution is symmetric at x- and z-direction and highest temperature is about 1404 °C.

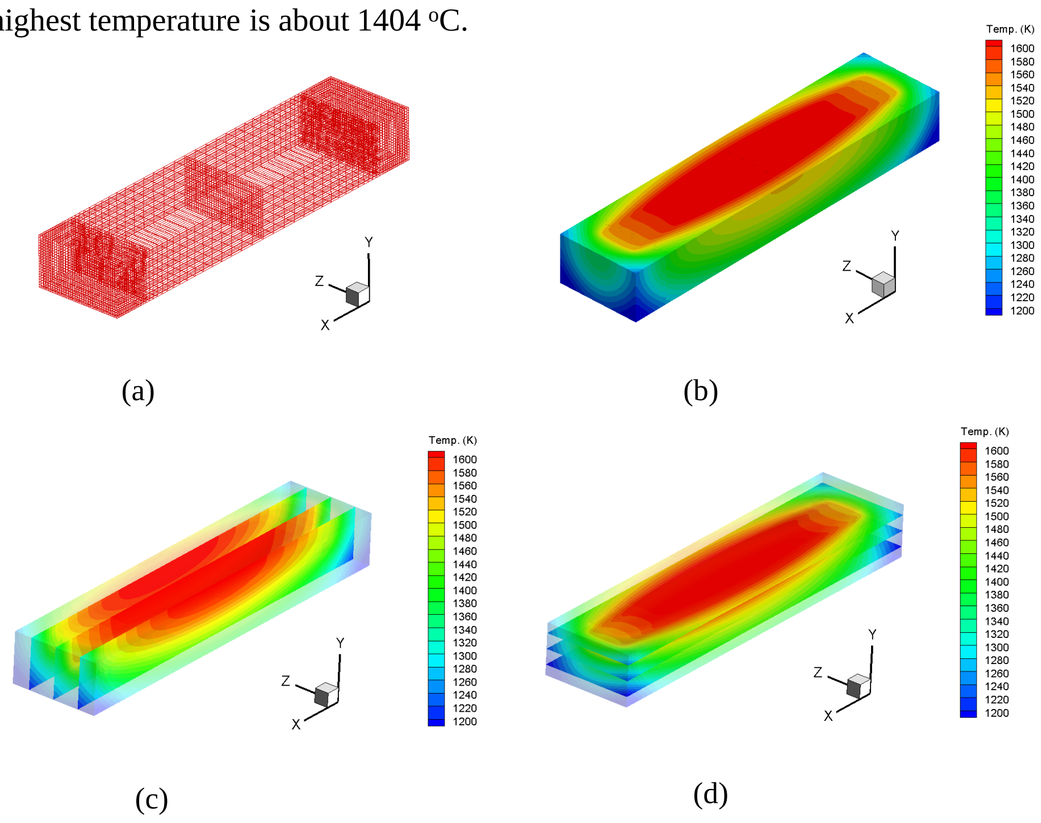

Figure 3: Simulation mesh and the temperature distribution of the copper ingot.

The computing domain and simulation results of the PDSC simulation are shown in Figure 4. Approximately 170,000 tetrahedral cells and 1.3 million simulated particles were used in the simulation. Three different kinds of particles are vaporized from different source ingots. The density and temperature decrease with increasing v-component velocity. The copper has higher values because it has highest number density and lightest molecular weight in this simulation.

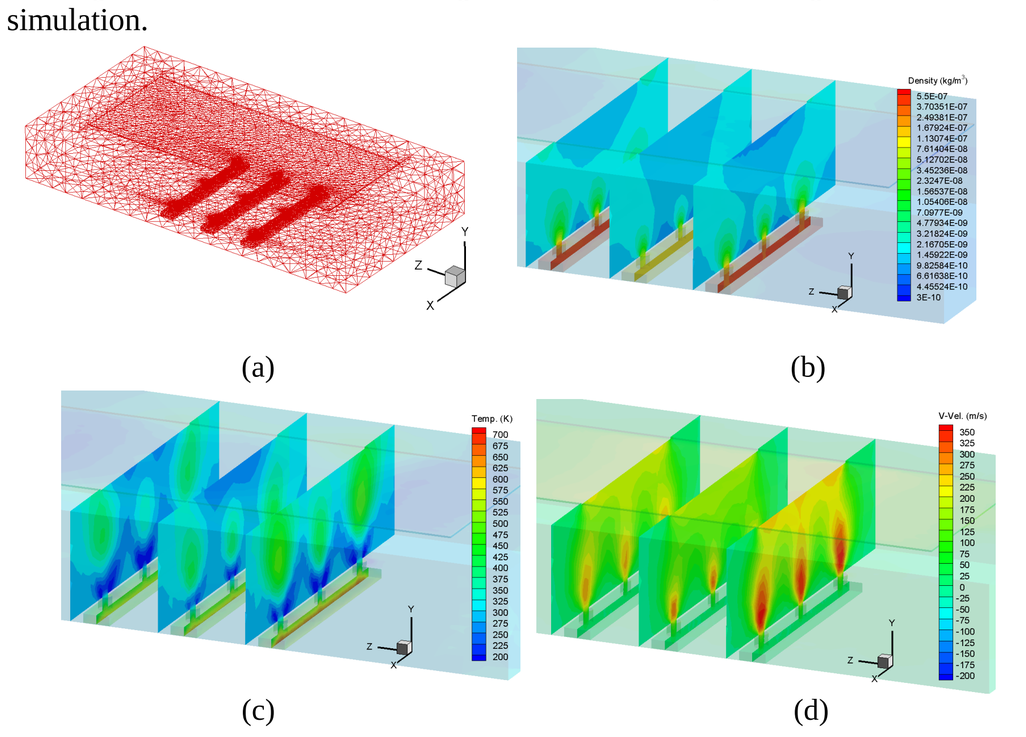

Figure 4: Simulation mesh and the contours of density, temperature and v-velocity.

Figure 5 shows the collected surface mass flux distributions, copper and gallium ratios. In a high-efficiency CIGS cell, the copper and gallium ratios are typically in the ranges of 0.8-0.9 and 0.25-0.4, respectively. These preliminary results can provide designers to tune parameters to meet the requirements.

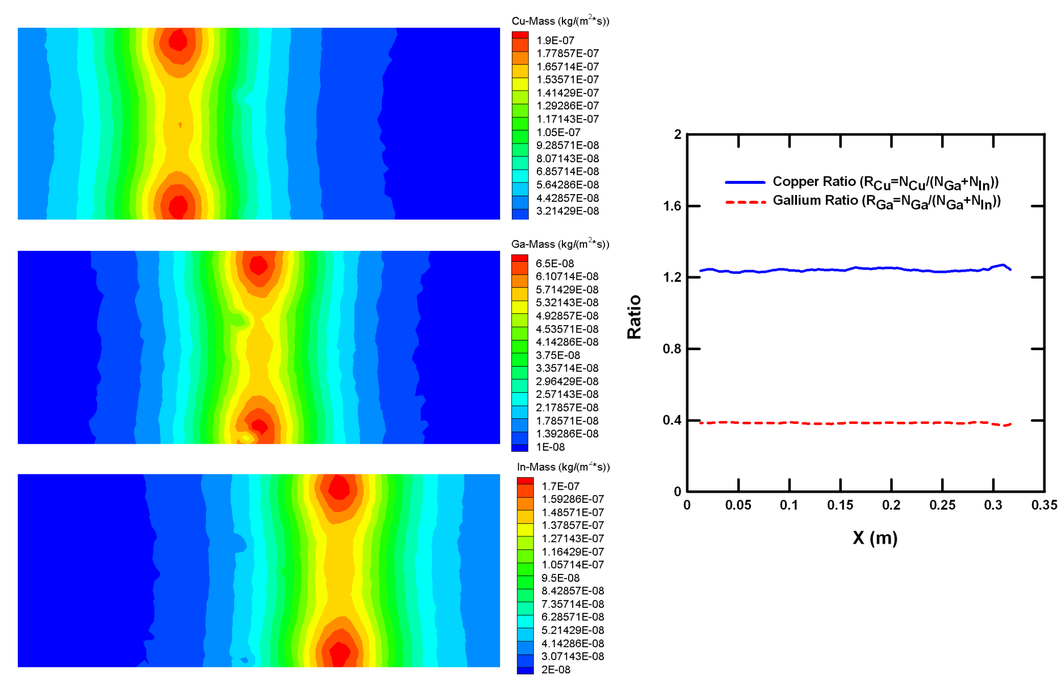

Figure 5: Simulated surface properties and the ratios of the copper and gallium ratios.

Conclusion

In the present study, a CIGS solar cell thin film deposition was simulated by proposed parallel hybrid simulation procedure. Results show that the method is able to simulate the deposition flux of various metal vapor on the glass. More parametric studies and improvement of the simulation speed are currently in progress.

Reference

1. Chen, Y.S., *7th International Conference on Finite Element Methods in Flow Problems*, Feb. 3-7, 1989, University of Alabama in Huntsville, Huntsville, Alabama.
2. Wu, J.-S.; Tseng, K.-C.; Wu, F.-Y.; *Comput. Phys. Comm.*, 2004, *162*, 166-187.
3. Kapil Mukati et al., *Ind. Eng. Chem. Res.* 2009, *48*, 5975–5991.