Florida Energy Systems Consortium

UNIVERSITY OF FLORIDA

A Low Cost CIGS Thin Film PV Process

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Description: PV has entered into a period of record growth. Most of the current production is based on crystalline Si technology. However, there are fundamental limits to the ultimate Si costs that may inhibit it from achieving the desired level of contribution to worldwide energy production. In contrast, thin-film PV technology can reach the desired outcome due to fast deposition rates and lower cost. Our study is focused on hot carrier solar cells for cell conversion efficiency improvement in a low cost, high throughput CIGS system. The rapid thermalizaton loss of hot photoexited carriers interacting with the lattice can potentially be reduced through phonon engineering in the absorber layer; the subsequent extraction of the hot carriers may be realized through device engineering of energy selective contacts.

Budget: $126,112.00

Universities: UF

Progress Summary

Research Objective-Low cost CIGS based hot carrier solar cells are studied for cell conversion efficiency improvement. To extract hot photo generated carriers, and thus achieve higher open circuited voltages, we plan on using phonon engineering in the absorber layer to slow the rate of carriers cooling and electrical engineering for optimizing energy selective contacts.

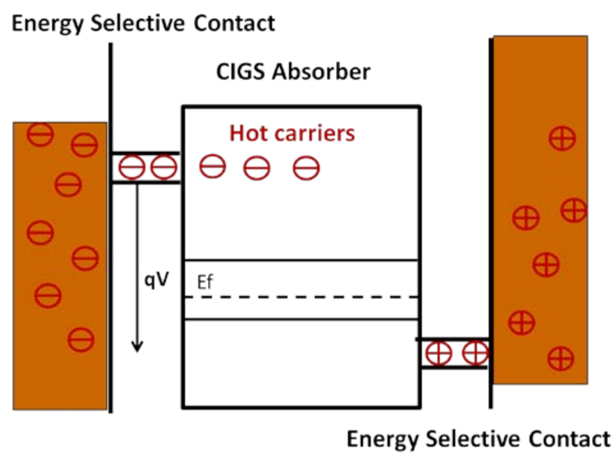

Figure 1. Schematic presentation of a hot carrier solar cell

Progress:

Phonon engineering in the absorber layer as presented in figure 1 was studied to reduce the hot carriers cooling rate. Hot carriers transfer their excess energy to the lattice in the form of optical phonons. Optical phonons are high-energy stationary lattice waves and are actually able to transfer energy back to the carriers to keep them hot. This slows down the net carrier cooling process. Typically an optical phonon decays into two, equal energy, acoustic phonons. This is called the Klemens mechanism. Acoustic phonons are low energy, propagating, waves. Once energy is in the form of an acoustic phonon, it cannot be recovered to re-heat carriers. Blocking the Klemens mechanism reduces the thermalisation of the hot carriers. This is achieved by phonon engineering via optimizing material composition and feature size which can lead to mini-gaps in the acoustic phonon branch and discreteness in the optical phonon branch, reducing the likelihood of optical phonon decay.

Device engineering of energy selective contacts as depicted in figure 1 is employed for the purpose of extracting hot carriers at the contacts without energy loss. The contacts are required to be very thin so that carriers can be collected before they interact with the lattice. The device design should allow collection of carriers at an optimal energy range. Carriers having energies outside this range will be rejected by the contacts to prevent energy loss. Quantum well structures such as resonant tunneling well/barrier diodes were used to design the energy selective contacts.

To focus on the absorber first, Fig. 2 shows the phonon dispersion curve for CIGS before and after phonon engineering. Black Solid lines represent the CGS bulk phonon dispersion curves. Red solid lines represent the CIS bulk phonon dispersion curves. The green, purple, and blue lines are the phonon dispersion curves for a super-lattice structure of 1 atomic layer of CIS over 2 atomic layer of CGS.

Phonon dispersion gives the relationship between phonon energy and wave vector. The bulk phonon dispersion curve is calculated by linear chain model, a simple "balls and springs" model for the atomic chain. The force on an atom depends linearly on the extension of its nearest-neighbor distances. Due to the connections between atoms, the displacement of one or more atoms from their equilibrium positions will give rise to a set of vibration waves propagating through the lattice.

In a superlattice structure, the acoustic branch phonon dispersion relationship is given by[1]

$$\cos(qD) = \cos(\frac{\omega d_A}{v_A})\cos(\frac{\omega d_B}{v_B}) - \frac{1+\delta^2}{2\delta}\sin(\frac{\omega d_A}{v_A})\sin(\frac{\omega d_B}{v_B}),$$

where $\delta = \frac{\rho_A v_A}{\rho_B v_B}$. Mini gaps appear in the acoustic branch where the blue lines disconnect. Optical phonon decay into acoustic phonons whose energy would fall into these gaps is forbidden since there is no allowed acoustic phonon state. The superlattice structure can be tuned, so that the mini-gaps are unfavorable for the Klemens decay to occur. In the optical branch, the wave vectors are limited to few possibilities due to confinement[2]. The corresponding wave numbers are discrete as well. Likewise the optical phonon branch of the superlattice becomes discrete, further reducing the probability of Klemens transitions. By carefully engineering the superlattice structure we can block or significantly reduce the Klemens mechanism and slow the carrier cooling rate.

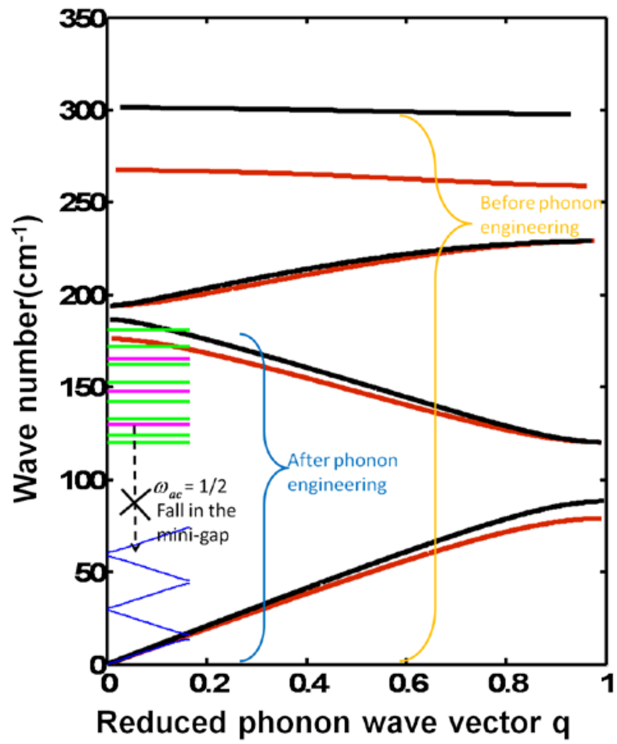

Figure 2. Phonon dispersion curves for bulk and superlattice structures

A double barrier quantum well structure was used to design the energy selective contact. Tunneling probability across barriers is calculated by using the transmission matrix[3]. $M = \prod_{l=0}^{N} M_l$,

$$M_l = \frac{1}{2}\begin{bmatrix} (1+S_l)\exp[-i(q_{l+1}-q_l)x_l] & (1-S_l)\exp[-i(q_{l+1}+q_l)x_l] \\ (1-S_l)\exp[i(q_{l+1}+q_l)x_l] & (1+S_l)\exp[i(q_{l+1}-q_l)x_l] \end{bmatrix},$$

where $S_l = \frac{m_{l+1}q_l}{m_l q_{l+1}}$ and q_l is wave vector. The transmission probability is given by $D(E) = \frac{m_0 q_{N+1}}{m_{N+1} q_0}|A_{N+1}|^2$, where

$$A_{N+1} = \frac{m_{N+1}q_0}{m_0 q_{N+1}}\frac{1}{M}.$$

The transmission current density is given by[4]

$$J(E_x)dE_x = \frac{qm_0}{2\pi^2\hbar^3} D(E_x, V_b) \times \int_{E_x}^{\infty} [f_0(E) - f_{N+1}(E)]dEdE_x$$. A Boltzmann distribution is assumed.

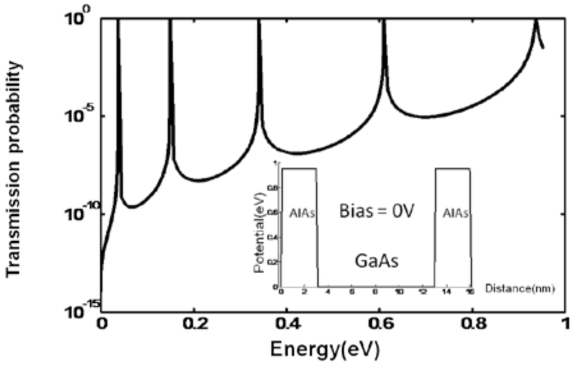

Figure 3. Tunneling transmission probability versus incoming electron energy at zero bias

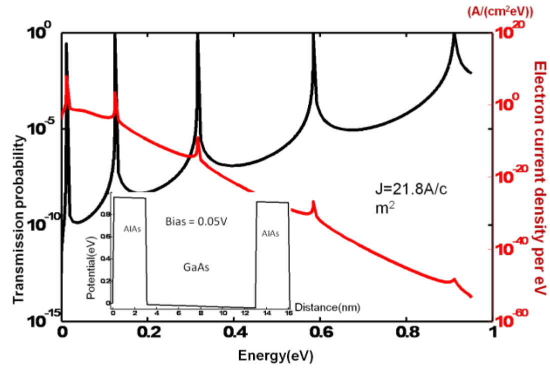

Figure 4. Tunneling probability and resulting current density as a function of incoming electron energy at a bias of 0.05V

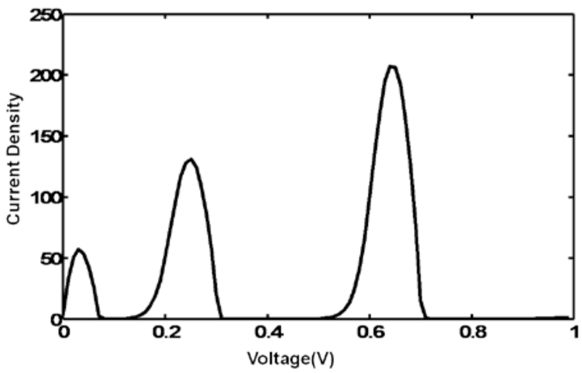

Figure 5. Current density versus applied bias of a double barrier tunnel diode

The quantum device studied is a 10nm GaAs well with 3 nm AlAs barriers. Fig. 3 is the transmission probability versus incident electron energy without any bias applied. We can see the energy selective property. In Fig. 4, a voltage of 0.05V is applied to the right hand side of the AlAs barrier. The transmission probability peaks appear at different incident electron energy due to the applied bias. The electron current density per eV (red curve) is plotted on the vertical axis on the right hand side. Fig. 5 gives the relationship of current density with voltage. There are discrete peaks showing how the current density varies as the voltage across the contact structure is changed. The transmission probability peaks shift—the tunneling state may no longer be a tunneling state at a slightly different bias. The carriers used to tunnel through now cannot tunnel through. The current density drops until a new tunneling state is reached at a higher voltage bias.

[1]:S.Tamura, D.C.Hurley, and J.P. Wolfe, "Acoustic-phonon propagation in superlattices", Phys. Rev. B 38(2) 1427-1449.
[2]:T. Dumelow, T.J. Parker, S.R.P. Smith and D.R. Tilley, "Far-infrared spectroscopy of phonons and plasmons in semiconductor superlattices", Surface Science Reports 17 (1993) 151-212.
[3]: Y. Ando and T. Itoh, "Calculation of transmission tunneling current across arbitrary potential barriers", J. Appl. Phys. 61(4) 1497-1502.
[4]: C.B. Duke, "Tunneling in Solids", Academic, New York, 1969.