

Metastability and Degradation of CdTe Solar Cells Investigated by nm-Scale Electrical Potential Imaging

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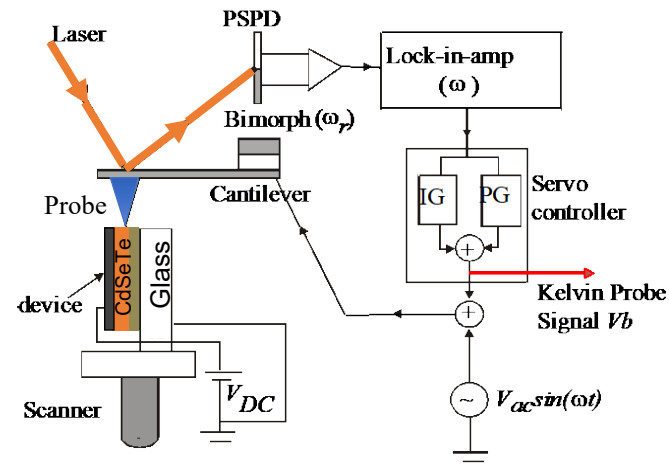
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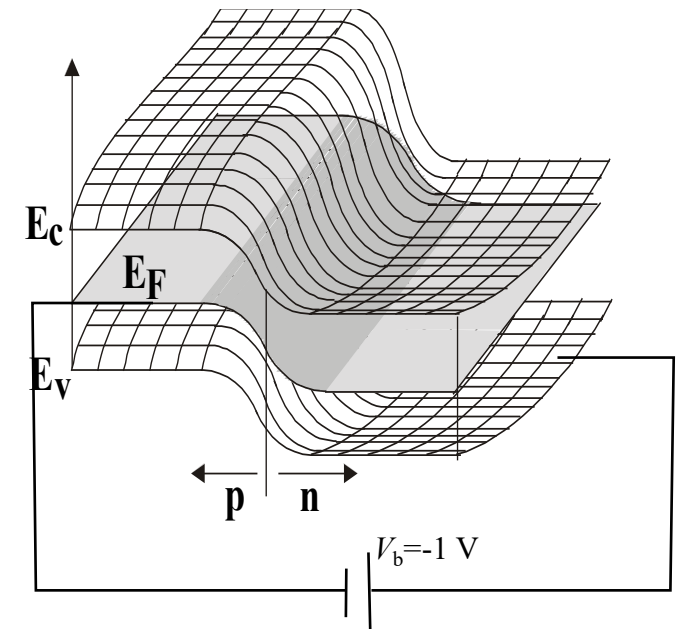
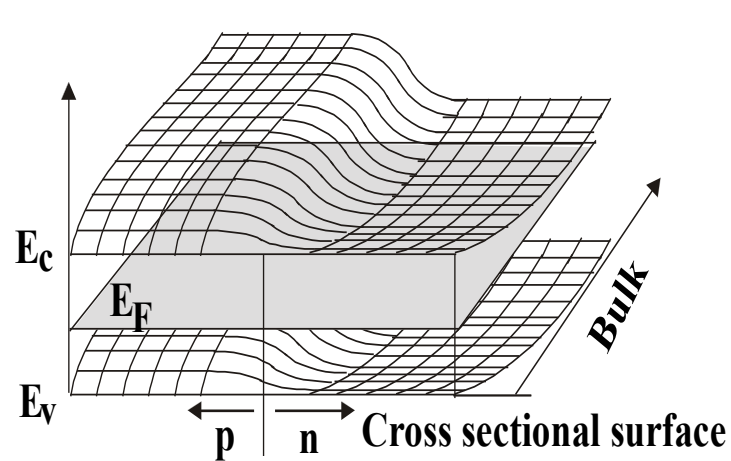
- **Brief introduction to KPFM potential imaging across PV devices**
- **CdSeTe Device metastability and degradation**
- **KPFM potential imaging at Dark-soak, light-soak, and degradation states**
- **Device modeling on electric field and J-V**
- **Summary**

KPFM potential imaging for PV junction structures

Kelvin probe force microscopy (KPFM)
Potential imaging by probing Coulomb force



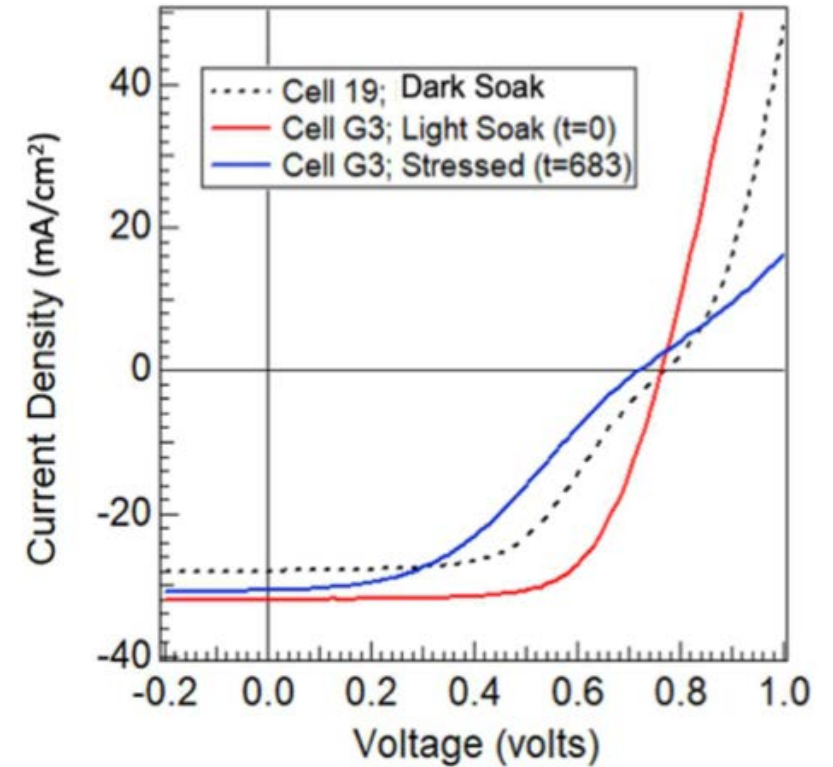
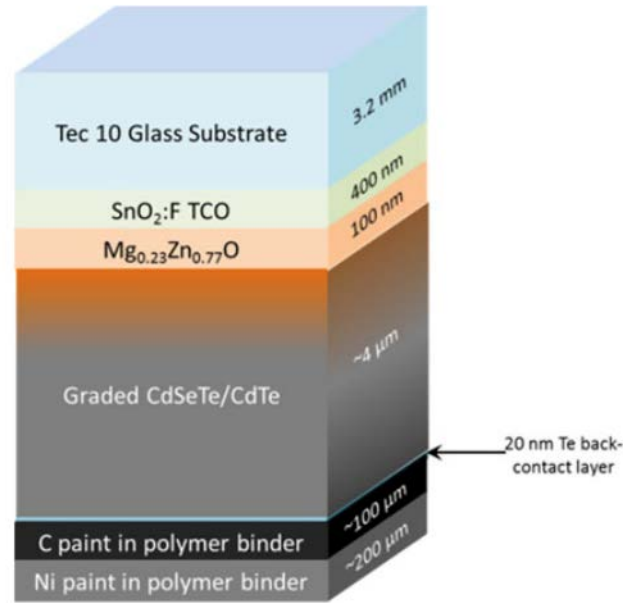
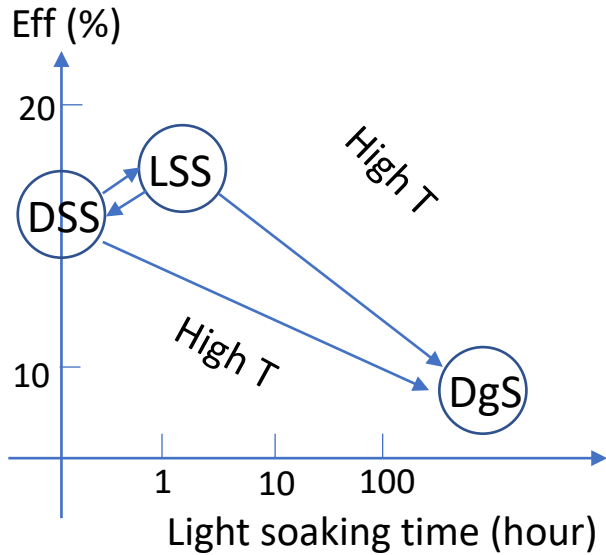
Junction location determined by surface potential profiling



- KPFM: **surface** potential imaging in ~ 30 nm spatial and ~ 10 meV energy resolutions
- Revealing bulk potential change by measuring surface potential change by applying a bias voltage (V_b) to the device
- Junction location determination in a normal single junction device by applying V_b , where the junction locates at the electric field peak
- More complicated device structure: KPFM measures the locations where external voltage drops or external field is added---usually need device modeling to reveal the device junction/barrier structures and carrier concentrations

Metastability and degradation of CdTe devices

Device structure A. Munshi et al., JPV 8, 310 (2018)



Dark-soak and light-soak states

| | Voc (V) | Jsc (mA/cm ²) | FF (%) | Efficiency (%) |
|------------|---------------|---------------------------|------------|----------------|
| Dark Soak | 0.757 ± 0.021 | 28.3 ± 1.0 | 55.8 ± 7.9 | 12 ± 2.0 |
| Light Soak | 0.780 ± 0.012 | 30.4 ± 0.8 | 70.4 ± 3.6 | 16.7 ± 1.2 |

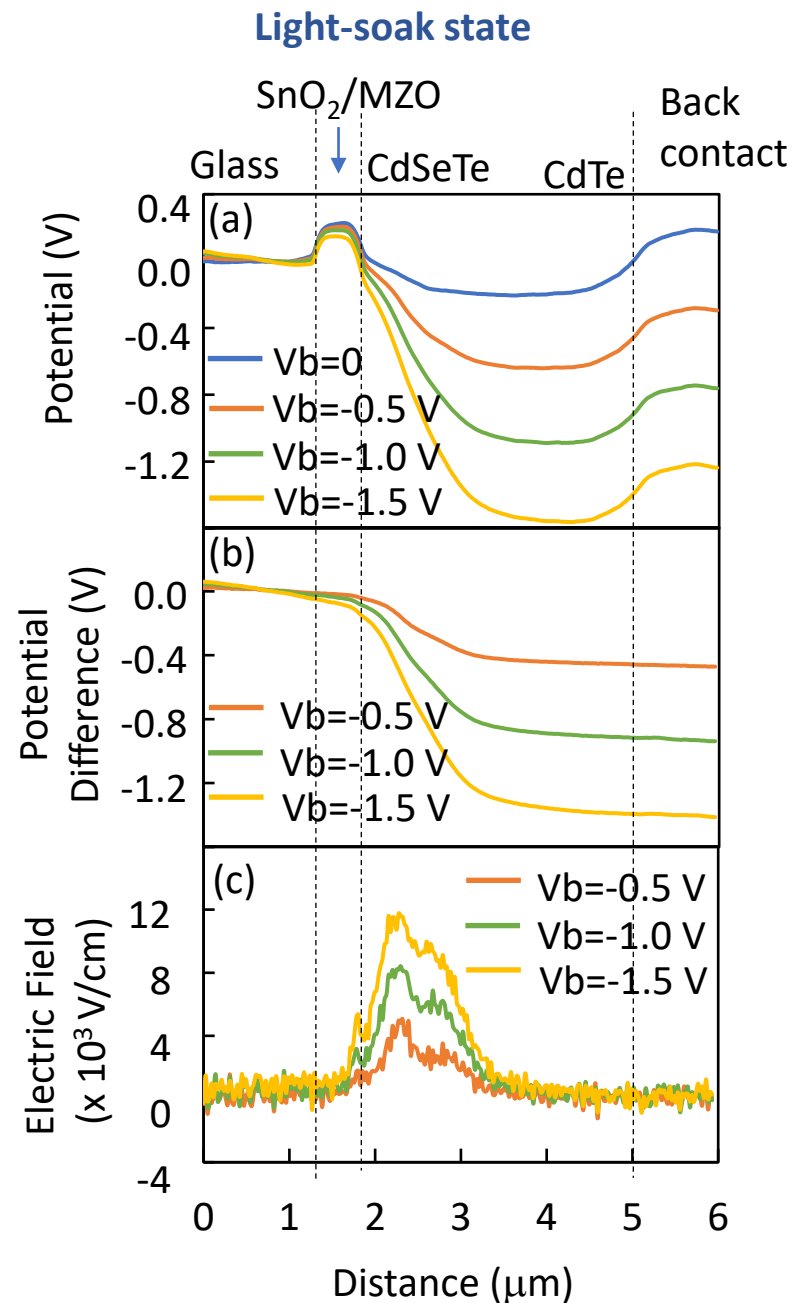
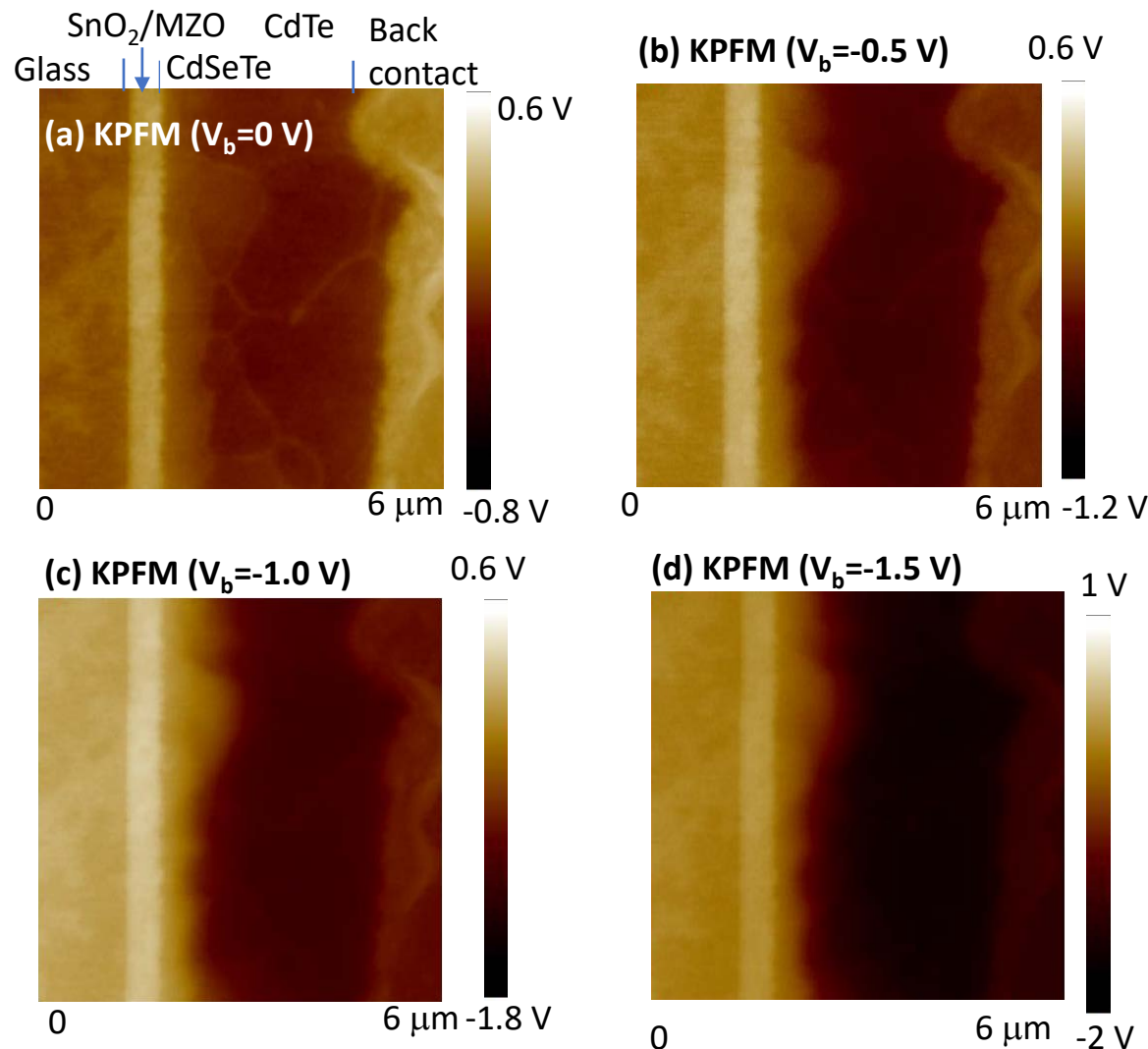
Light-soak and degradation states

Device performance parameters at the DgS after light-soaking at one sun at 65 °C for 683 h.

| Time (hrs) | Voc (V) | Jsc (mA/cm ²) | FF (%) | Efficiency (%) |
|------------|---------|---------------------------|--------|----------------|
| 0 | 0.756 | 30.3 | 66.3 | 15.2 |
| 683 | 0.722 | 29.7 | 44.3 | 9.5 |

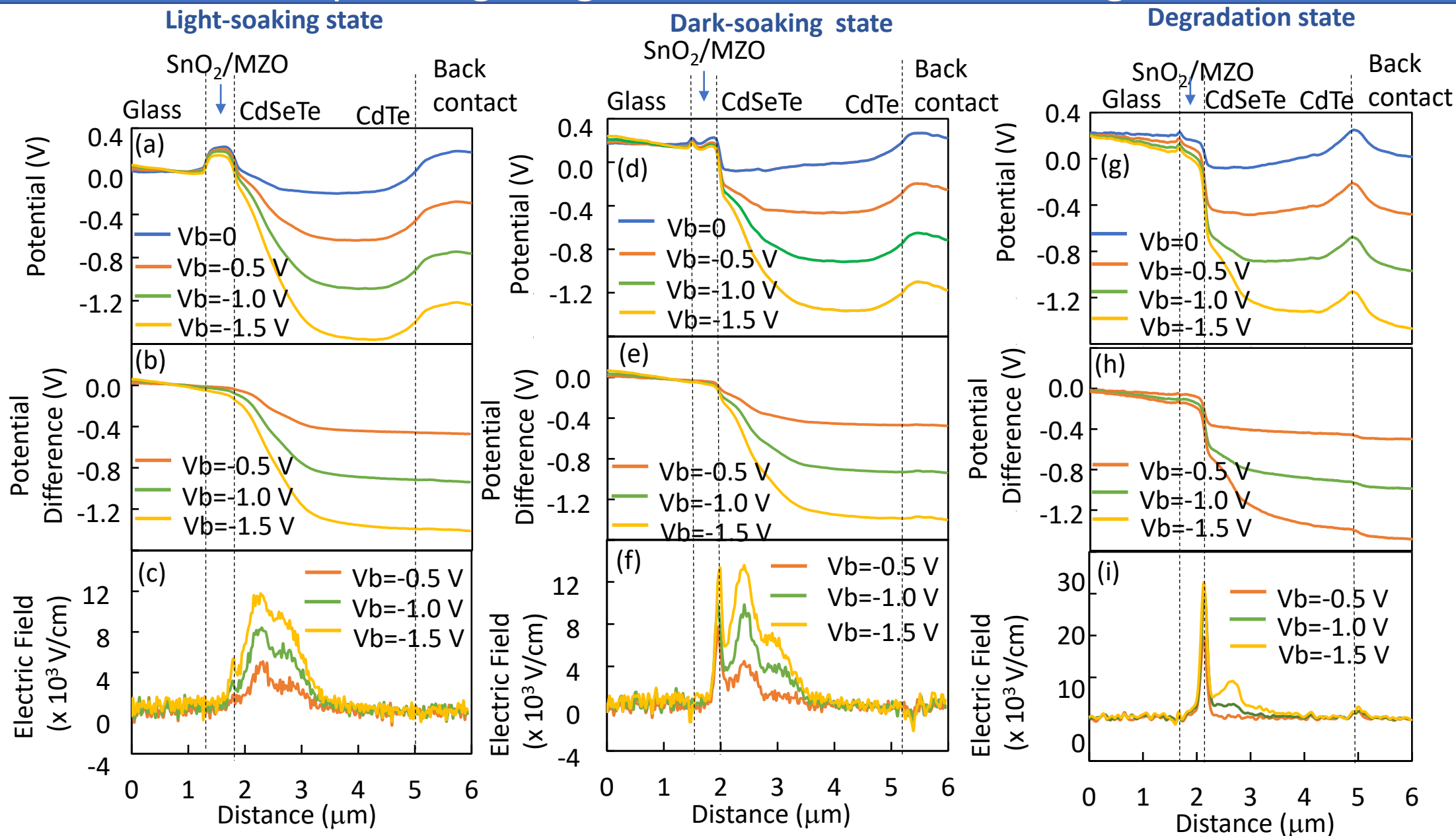
- FF degradation dominates the performance change in both dark-soak and degradation states
- The devices were with spray back metallization, devices with sputtered metallization show much less change with stressing

KPFM potential imaging at light-soak state with various V_b



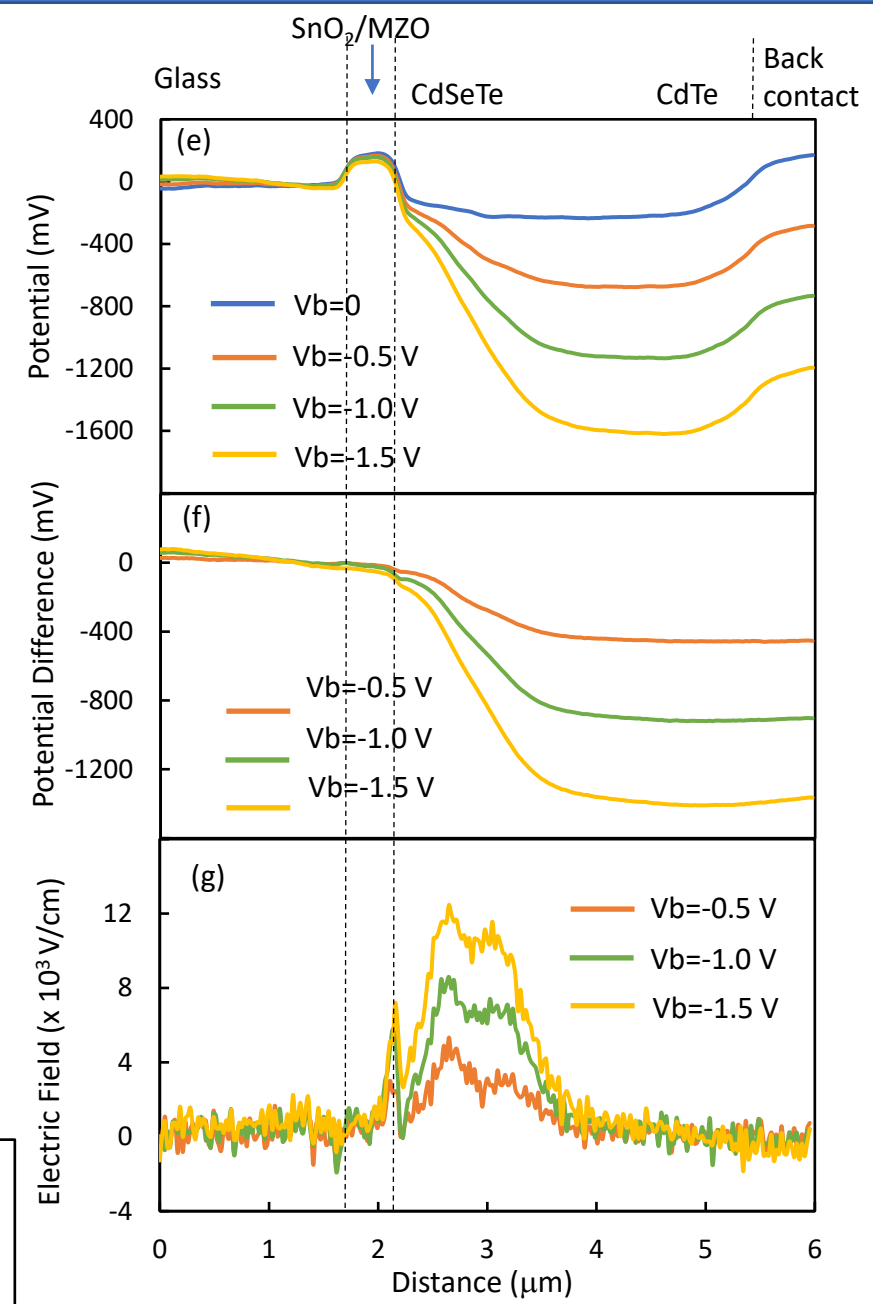
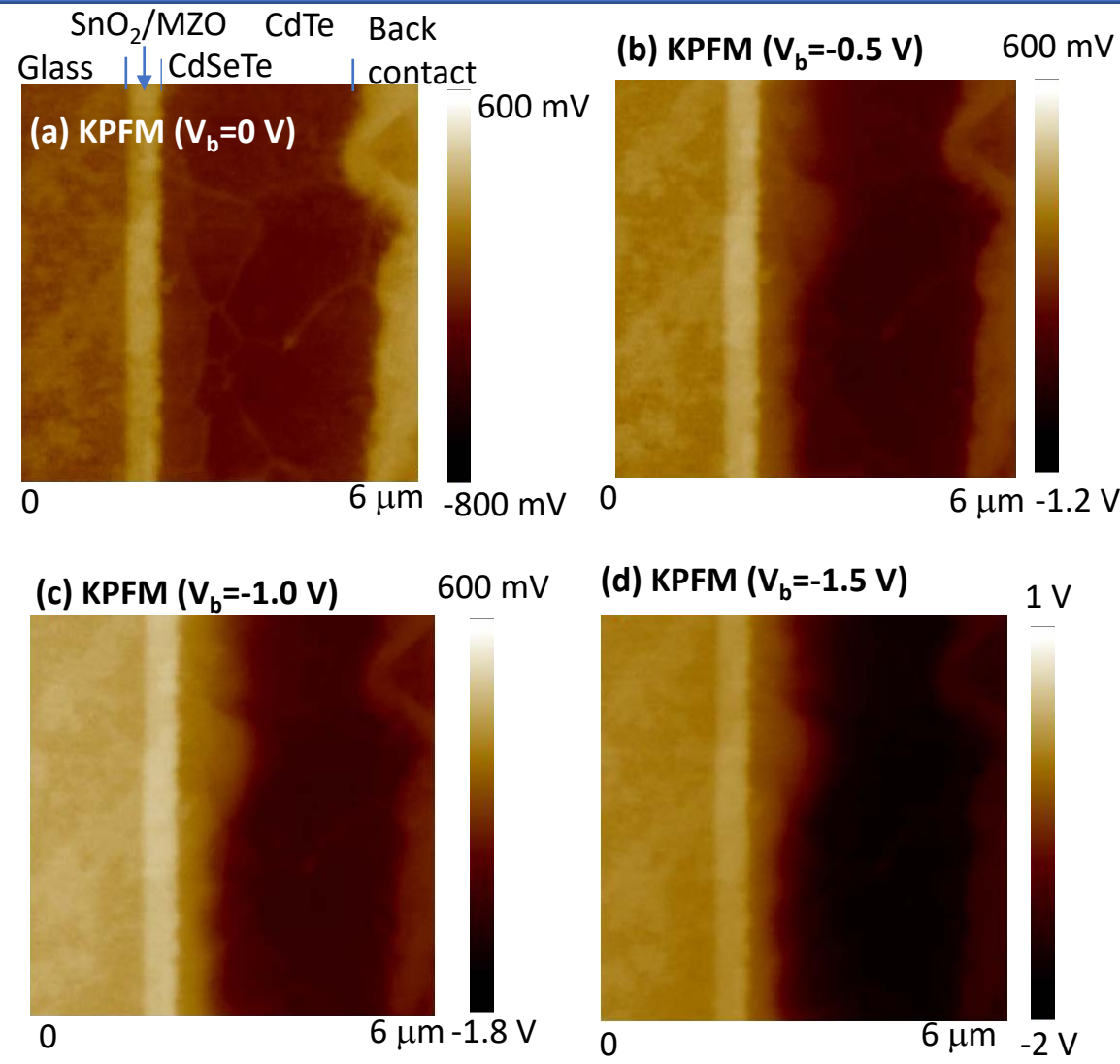
- KPFM measurement at dark and room temperature
- The main electric field is within CdSeTe layer, not at the MZO/CdSeTe interface: a buried homo-junction (BHJ)
- There is a small electric field at the MZO/CdSeTe interface at the light-soak state

Potential/field profiling at light-soak, dark soak, and degradation states



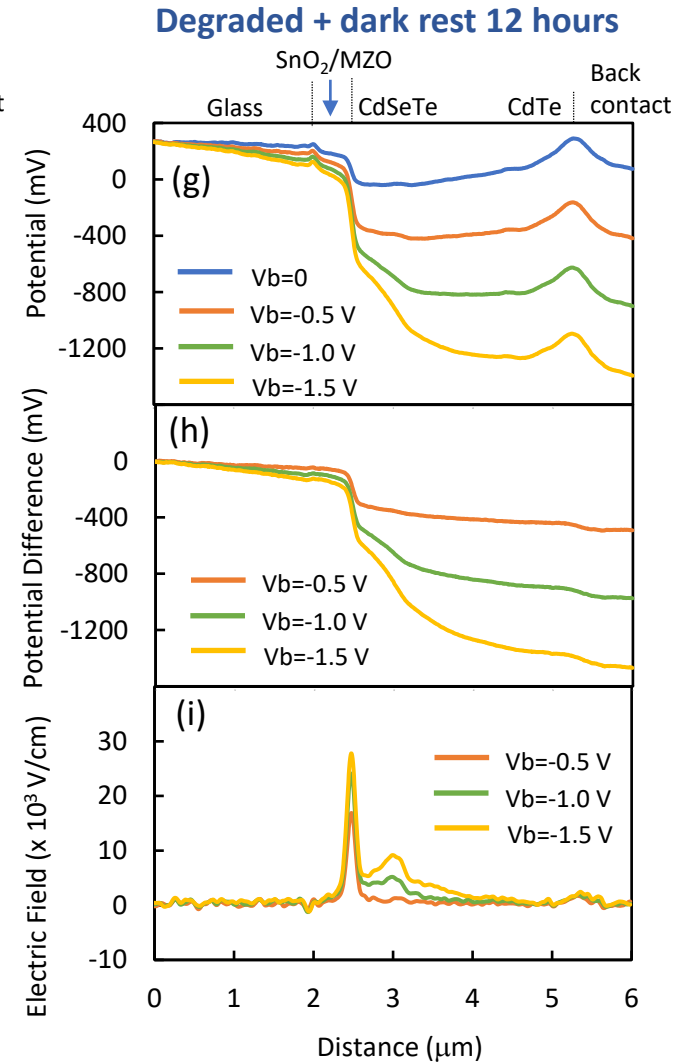
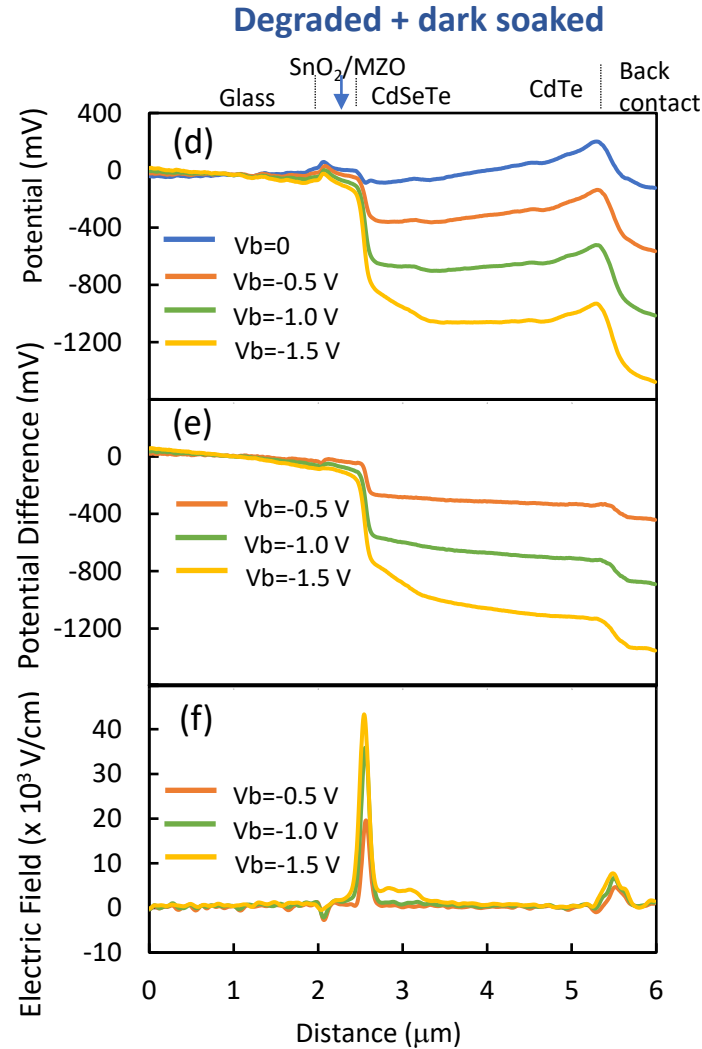
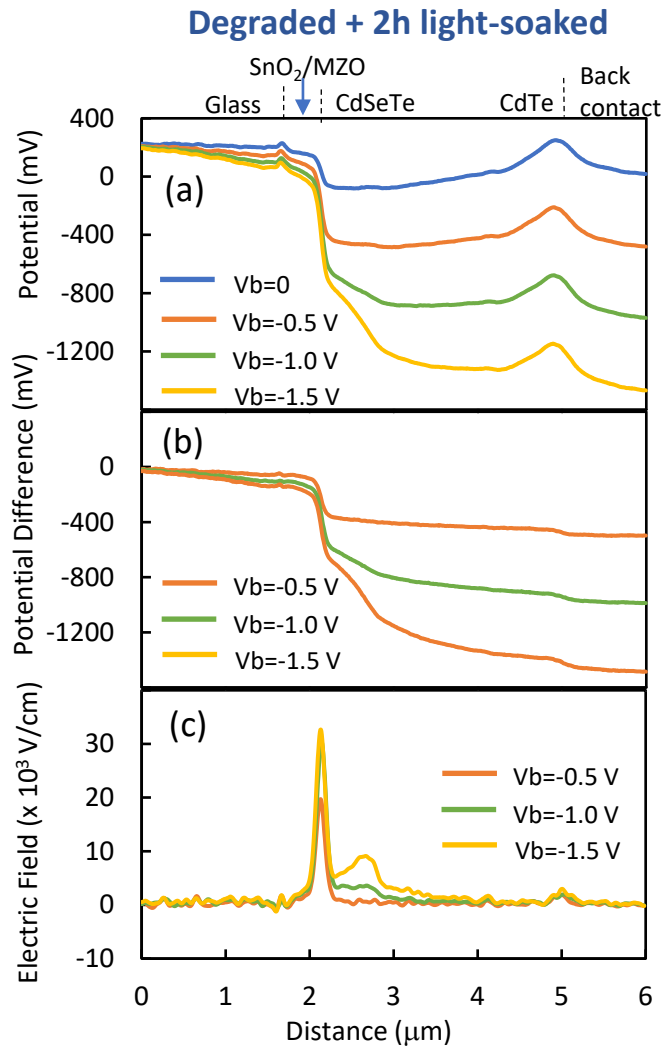
Double electric field peaks at dark-soak state; the peak at the interface further increased at degradation state and a small field at the back appeared

Electric field at intermediate dark rest state---metastable electric field



- Dark state was measured 24 hours after dark soak
- At dark rest 12 hours, the electric field at the MZO/CdSeTe interface increased to the halfway, verified the metastable electric field

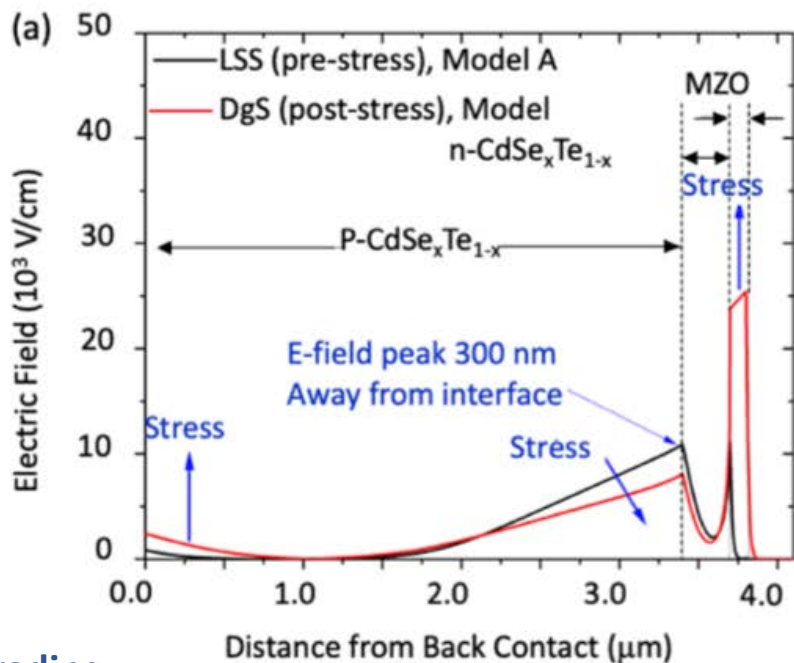
Electric field at degradation state with light-soak and dark soak---stable and irreversible degradation state



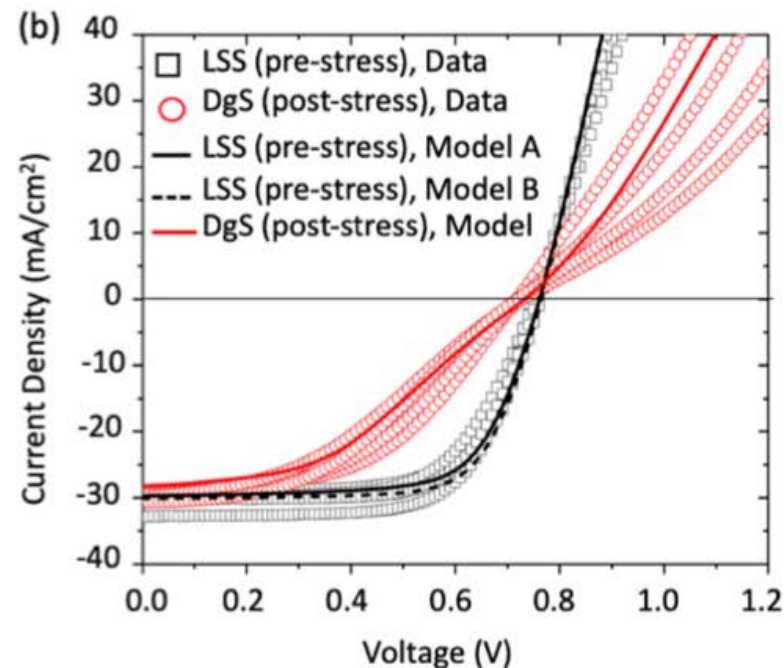
No significant change in electric field by light soaking, dark soaking, and dark rest--- the degradation state is stable and irreversible

Device modeling for light-soak and degradation states

Electric field



Experimental and modeled J-V



Bandgap grading

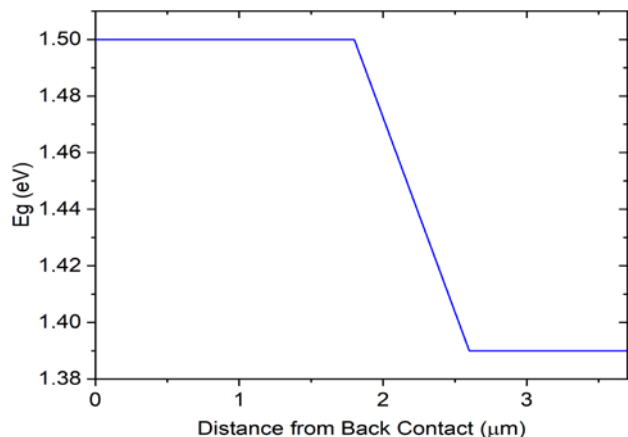


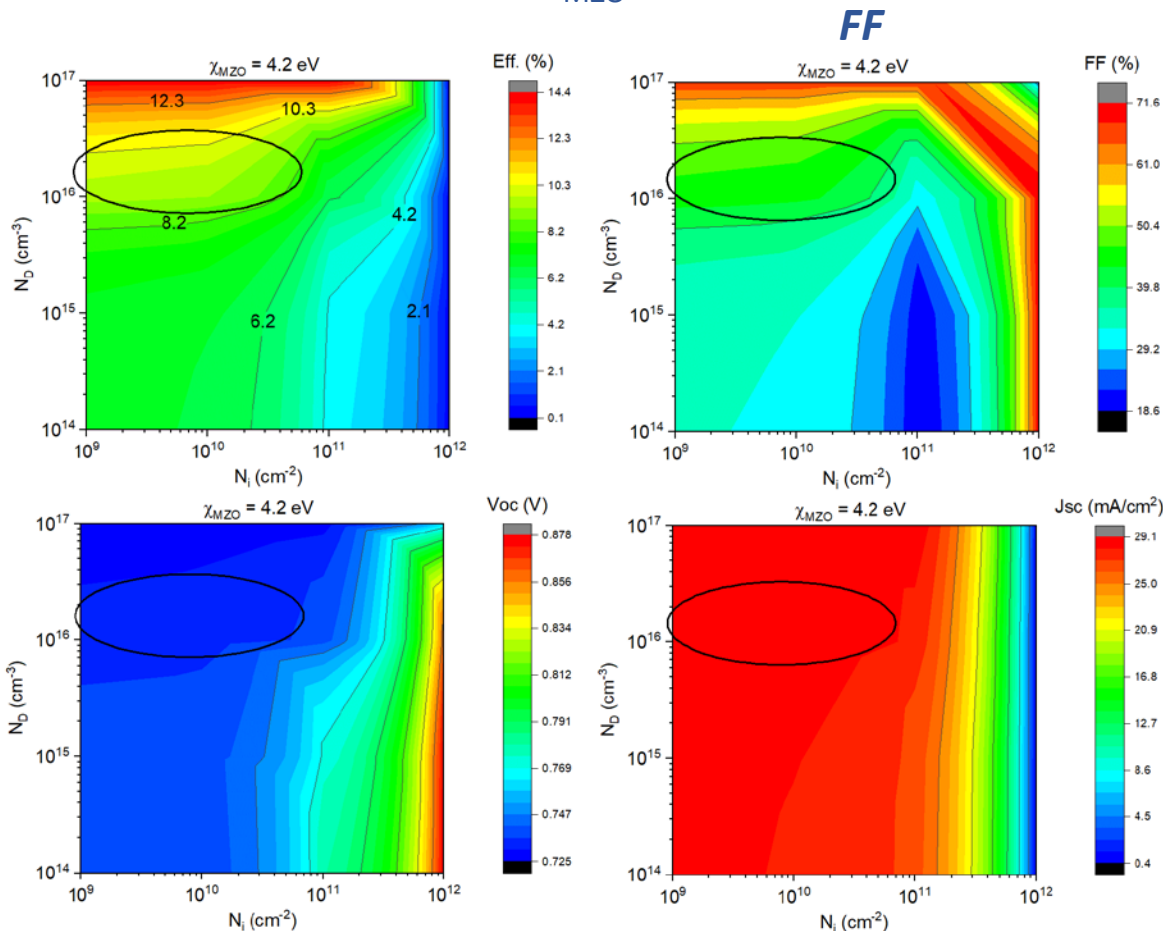
Table S1. Baseline device model parameters [1]-[4].

| Parameter | Symbol | Unit | SnO ₂ :F | Mg(Zn,O) | p-Cd(Se,Te) | n-Cd(Se,Te) |
|-------------------|------------------|---------------------|---------------------|---------------------|-----------------------|-----------------------|
| Thickness | h | nm | 400 | 100 | 3,400 | 300 |
| Band Gap | E_g | eV | 3.6 | 3.75 | 1.5–1.39* | 1.39 |
| Rel. Permittivity | ϵ | | 9.0 | 9.0 | 9.4 | 9.4 |
| Electron Affinity | χ | eV | 4.4 | 4.49 | graded* | 4.49 |
| Mobility | μ_n, μ_p | cm ² /Vs | 100, 25 | 1, 25 | 320, 40 | 320, 40 |
| Lifetime | τ_n, τ_p | ns | 0.1, 0.1 | 0.1, 0.1 | 2, 2 | 2, 2 |
| Doping | N_A, N_D | cm ⁻³ | n: 10 ¹⁷ | n: 10 ¹⁴ | p: 4x10 ¹⁴ | n: 4x10 ¹⁵ |

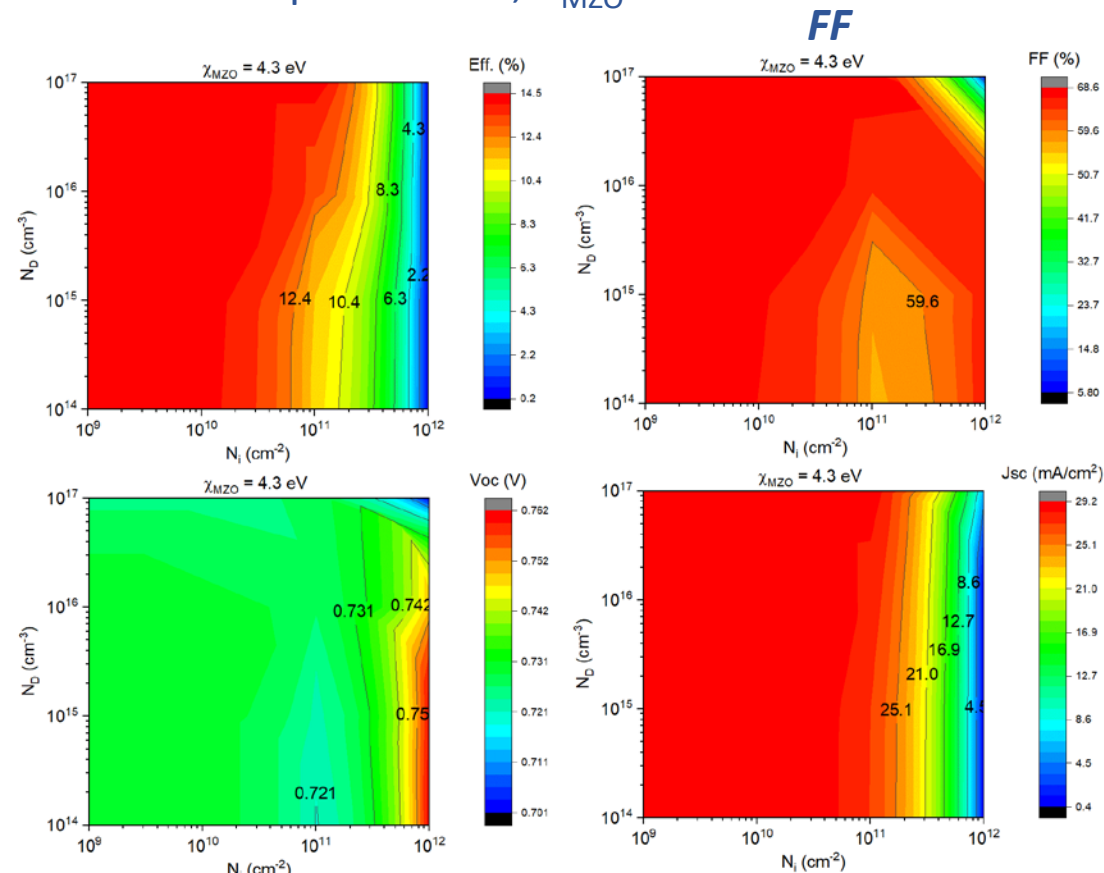
Device modeling using COMSOL Multiphysics software in alignment with J-V and electric field
 J-V: dominantly FF loss; Electric field: increasing around MZO

Device modeling for light-soak and degradation states

Spike=0.3 eV, $\chi_{\text{MZO}}=4.2$ eV



Spike=0.2 eV, $\chi_{\text{MZO}}=4.3$ eV



- Parameter space: band offset, MZO doping, Interface defect density N_i
- Light soak state: either MZO doping is good ($>10^{18}/\text{cm}^3$) or small band alignment spike <0.3 eV ($\chi_{\text{MZO}} > 4.2$ eV). Model A for LSS: spike=0.3 eV, $N_{\text{MZO}}=10^{18}/\text{cm}^3$, $N_i=10^9/\text{cm}^2$, Model B: spike=0, $N_{\text{MZO}}=10^{14}/\text{cm}^3$, $N_i=10^9/\text{cm}^2$
- Degradation state, both poor doping ($<10^{16}/\text{cm}^3$) and large band spike >0.2 eV, DSS in graph: spike=0.3 eV, $N_{\text{MZO}}=10^{16}/\text{cm}^3$, $N_i=10^9/\text{cm}^2$; based on literature (Pandy et al., SOLMAT 232 (2021), 111324), the doping decrease at a large spike is more plausible?

Summary

- **KPFM surface potential imaging: 30 nm spatial and 10 meV energy resolutions**
- **KPFM potential profiling across devices: nm-resolution junction location determination (buried homojunction for the CdSeTe device), junction/barrier structure for more complicated device than normal single junction device etc.**
- **Metastability and degradation of CdSeTe devices: additional electric field at MZO/CdSeTe interface for both dark state and degradation state.**
- **Device modeling in alignment with both the electric field and J-V: The degradation can be induced either by MZO doping (D_{MZO}) decrease at a large MZO/CdSeTe band offset spike or an offset spike increase at low D_{MZO} .**

Thank you

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