Role of light and heavy alkalis in $Cu(In,Ga)Se_2$ solar cells

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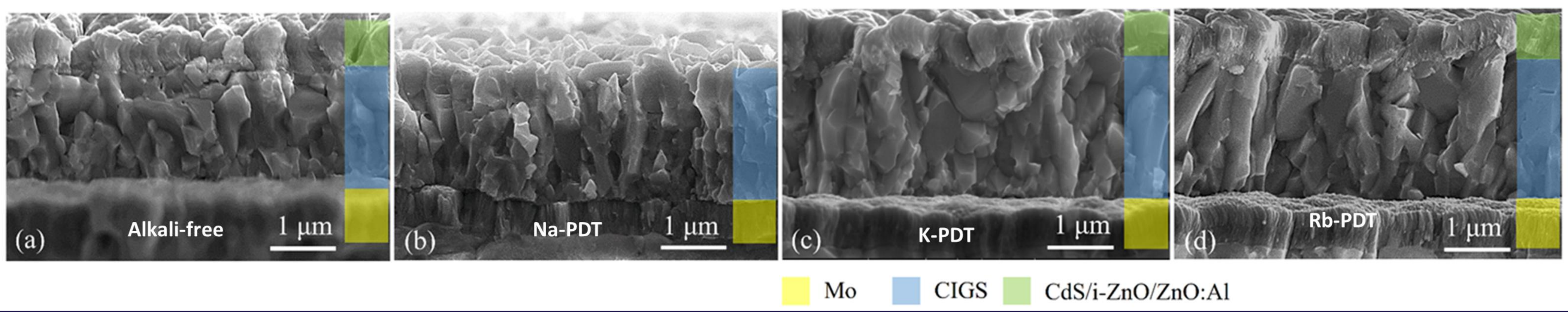
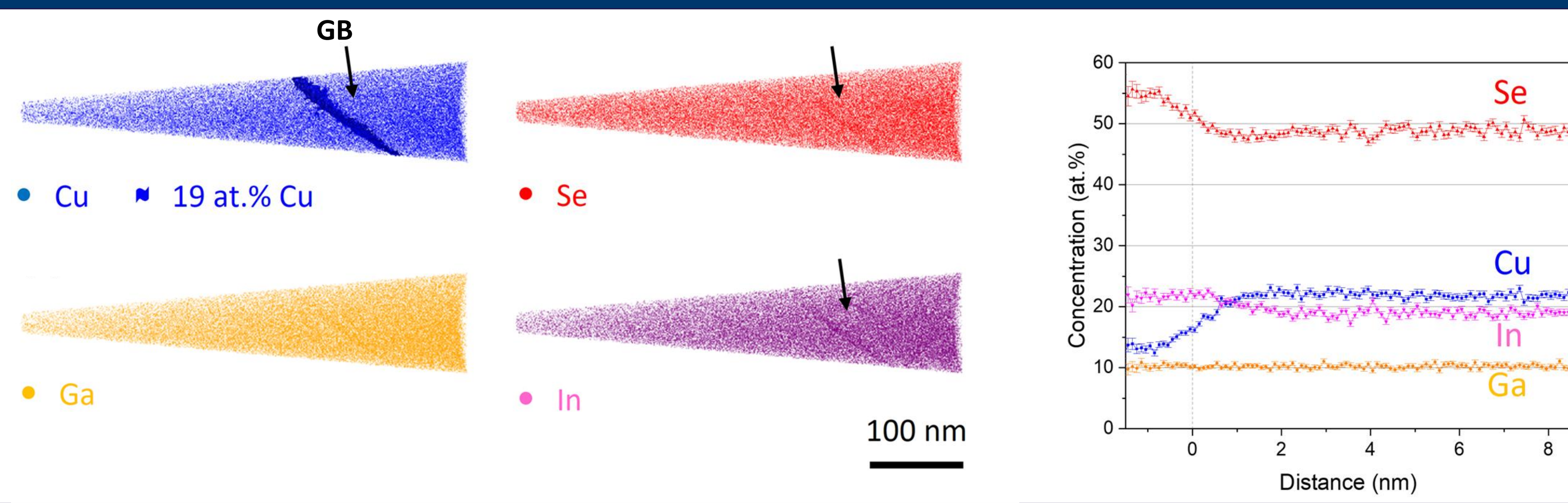
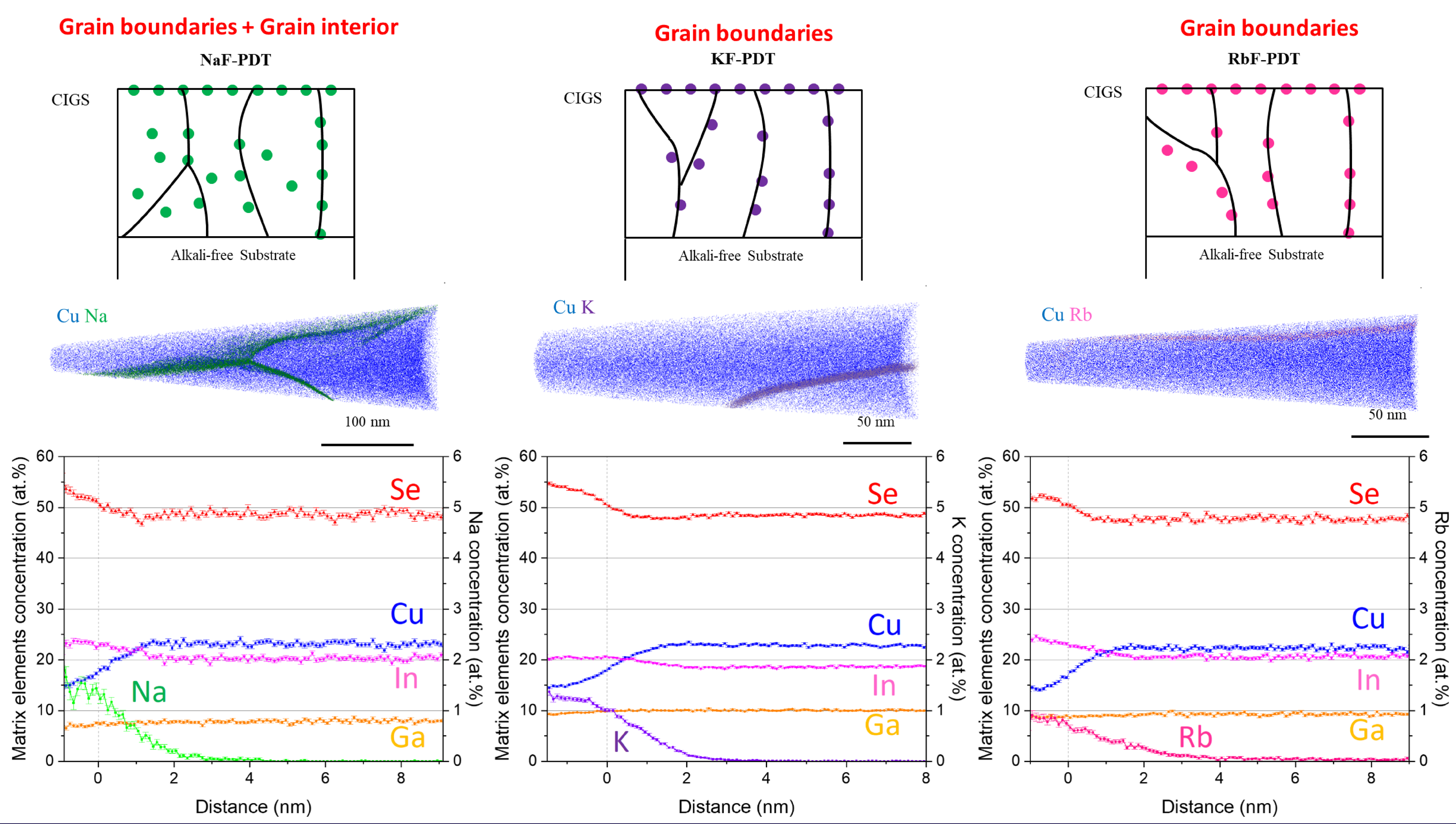
Samples: Na, K, Rb-doped CIGS absorbers



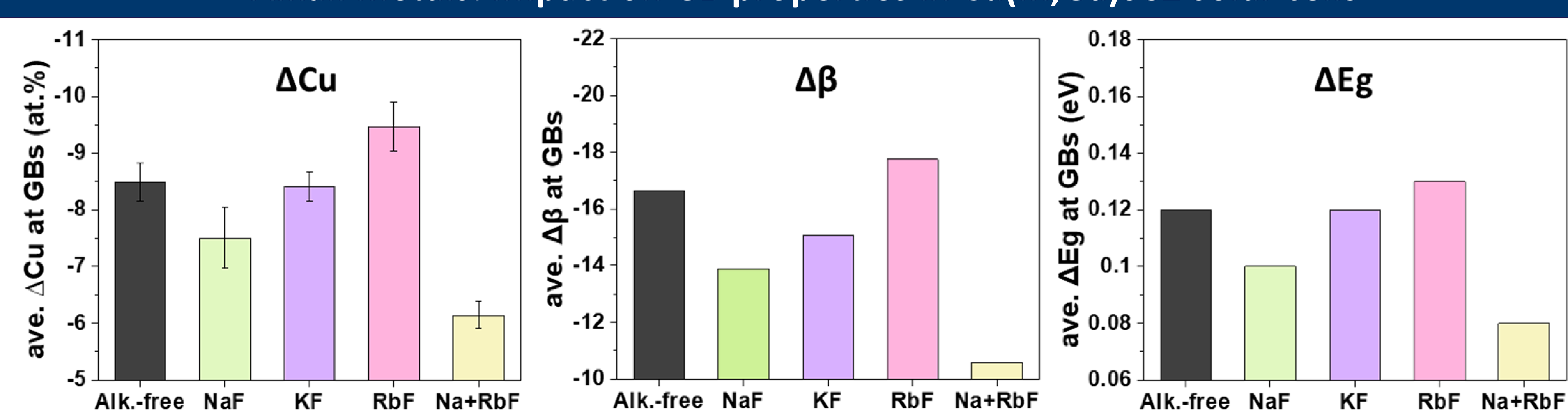
Grain boundaries in alkali-free absorbers

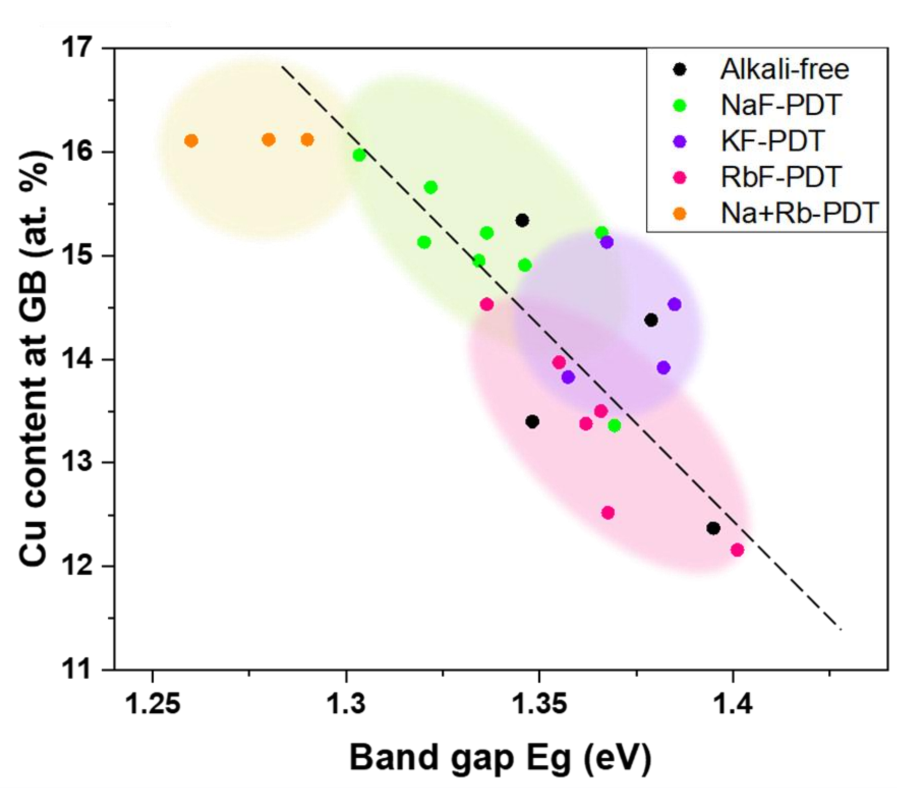


Grain boundaries in alkali-containing absorbers



Alkali metals: impact on GB properties in Cu(In,Ga)Se2 solar cells





- $\Delta\beta = \Delta Cu - (\Delta Se + \Delta In + \Delta Ga)$
- Magnitude of $\Delta\beta \Longleftrightarrow$ Degree of **donor-type**
  - Detrimental GBs, Cu-enriched GBs, positive values, acceptor defects are dominant
  - Beneficial GBs, Cu-depleted GBs, negative values, donor defects are dominant
- $E_g = (1-x)E_g^{CIS} + xE_g^{CGS} - bx(1-x) + \alpha(25 - X_{Cu})$
- **Average ΔE_g**: the difference between the band gap of the GB and that of the bulk increases from the GBs of the Na+RbF-PDT sample to the GBs decorated with Rb

Introduction

- Understanding the beneficial role of doped alkali elements in enhancing the efficiency of $Cu(In,Ga)Se_2$ (CIGSe) absorbers
- Deeper insights into defect states in the absorber, particularly near grain boundary (GB) regions.
- Distribution of light and heavy alkali metal dopants (Na, K, and Rb) is investigated at GBs and within the bulk with sub-nanometer resolution.

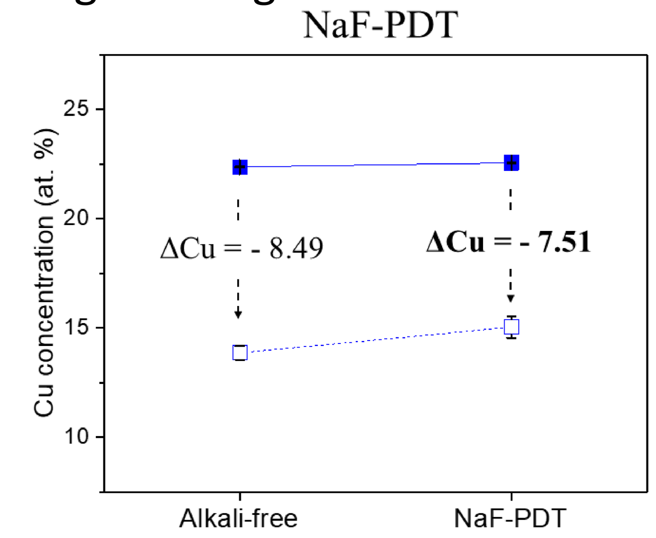
Methods

- A correlative microscopy approach:
  - Atom probe tomography (APT)
  - Electron backscatter diffraction (EBSD)

Results

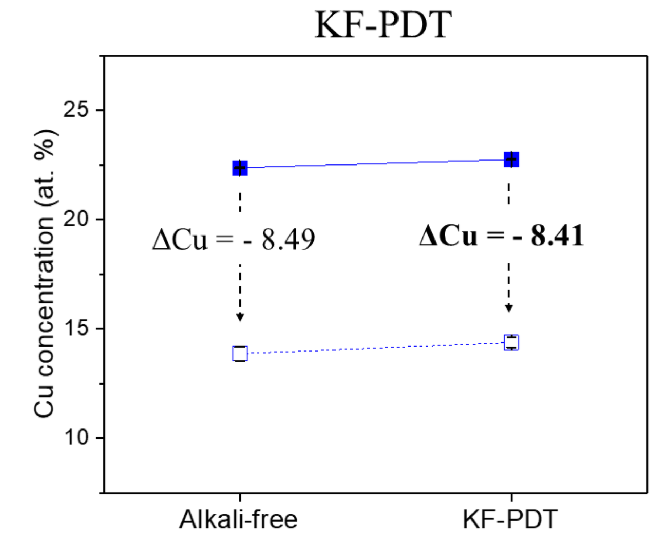
- Compositional fluctuations of both matrix elements and doped alkali elements between the bulk and grain boundaries (GBs) upon doping
- Correlation between alkali element concentration and In enrichment at GBs, which is attributed to the formation of donor-type defects.
- We propose possible mechanisms governing the distribution of Cu:

NaF-PDT



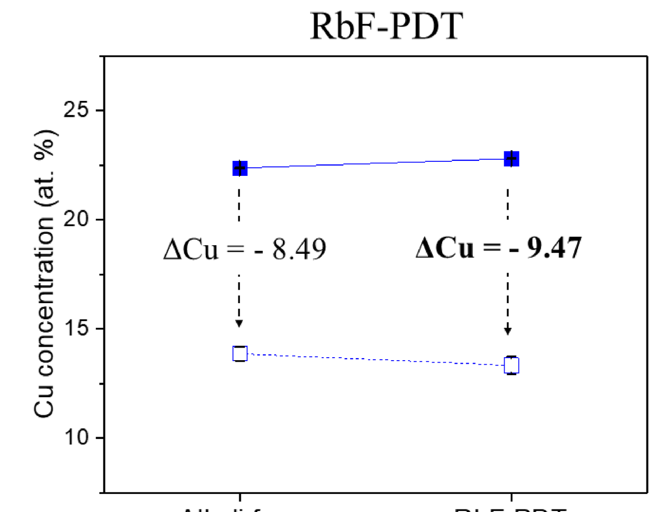
- Reduces ΔCu
- Cu atoms flow toward GBs

KF-PDT



- ΔCu almost unchanged
- Flows in both direction?

RbF-PDT



- Increases ΔCu
- Cu atoms flow out of GBs

Discussion

- NaF- and KF-PDT, less negative Δβ in average, GBs are less n-type
- RbF-PDT, more negative Δβ in average, GBs are more n-type

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