# On the effects of impurities and defects on GaAs-based photovoltaics

*Thales Borrely[1, 2], Ahmad Alzeidan[2], Alain A. Quivy[2], Gabriel M. Jacobsen[3], Marcio D. Teodoro[3], Raja R. S. Gajjela[4], Arthur L. Hendriks[4], and Paul M. Koenraad[4]

[1]University of Michigan

[2]University of São Paulo

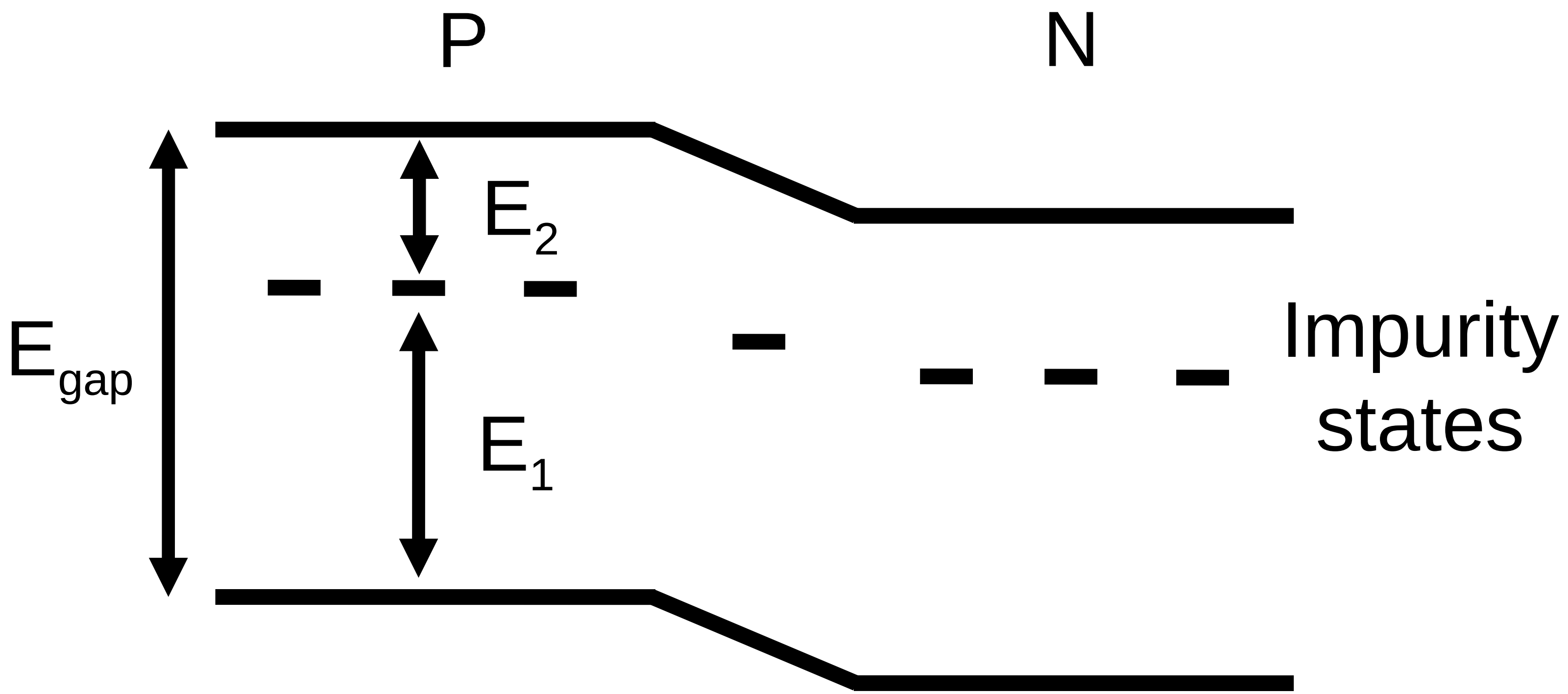
[3]Federal University of São Carlos

[4]Eindhoven University of Technology

*email: thales.santos@usp.br / thaless@umich.edu

# Impurity solar cells

- Absorption and current enhancement[1]
- Recombinations increase and voltage loss[2]





[1] M. Wolf, Limitations and Possibilities for Improvement of Photovoltaic Solar Energy Converters, Proc. of the IRE 48 (1960) 1246.
[2] W. Shockley, H. J. Queisser, Detailed Balance Limit of Efficiency of p-n Junction Solar Cells, J. Appl. Phys. 32 (1961) 510.

# Impurity photovoltaic effect

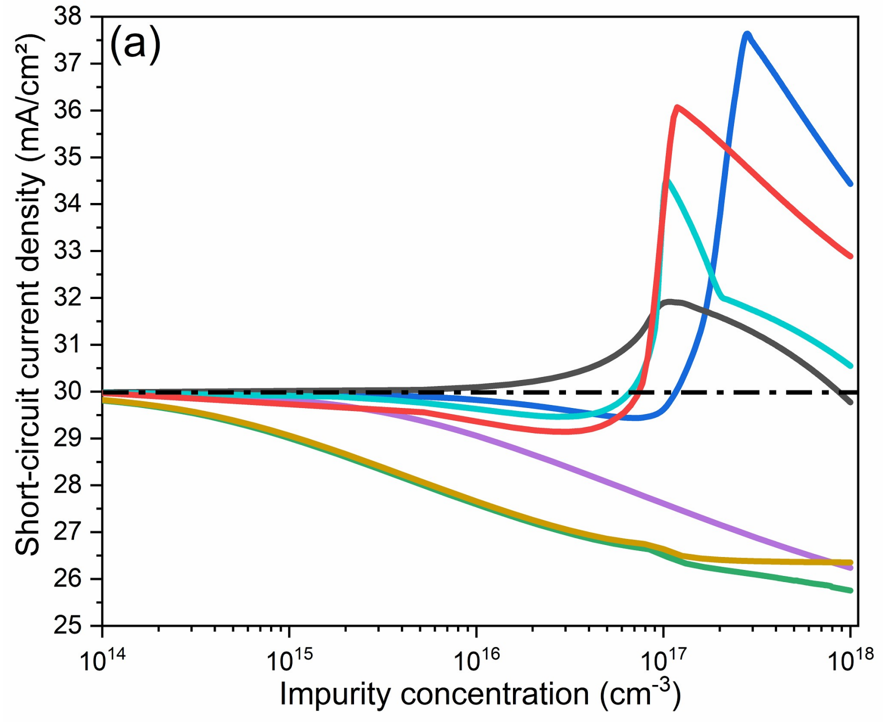
- 1990s and 2000s: a few studies on Si-based impurity solar cells, mostly theoretical using a modified SRH recombination model[1].

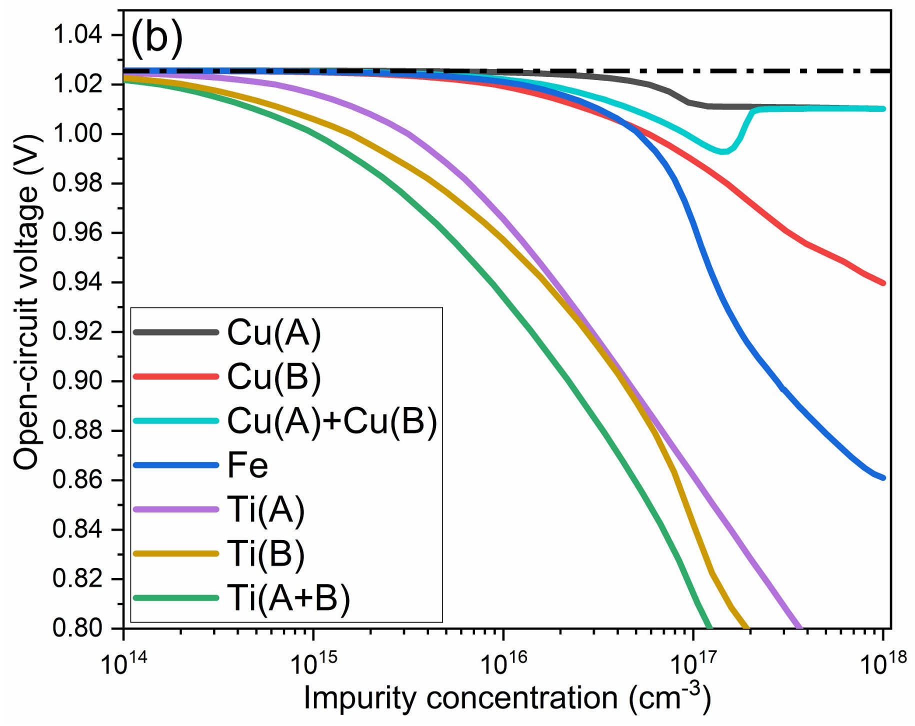
$$U = \frac{np - (n_1 + \tau_{n0} g_{nt})(p_1 + \tau_{p0} g_{pt})}{\tau_{n0}(p + p_1 + \tau_{p0} g_{pt}) + \tau_{p0}(n + n_1 + \tau_{n0} g_{nt})}$$

- Epitaxial materials were left behind.

[1] M. J. Keevers, M. A. Green, Efficiency improvements of silicon solar cells by the impurity photovoltaic effect, J. Appl. Phys. 75 (1994) 4022

# GaAs-based impurity solar cell simulations

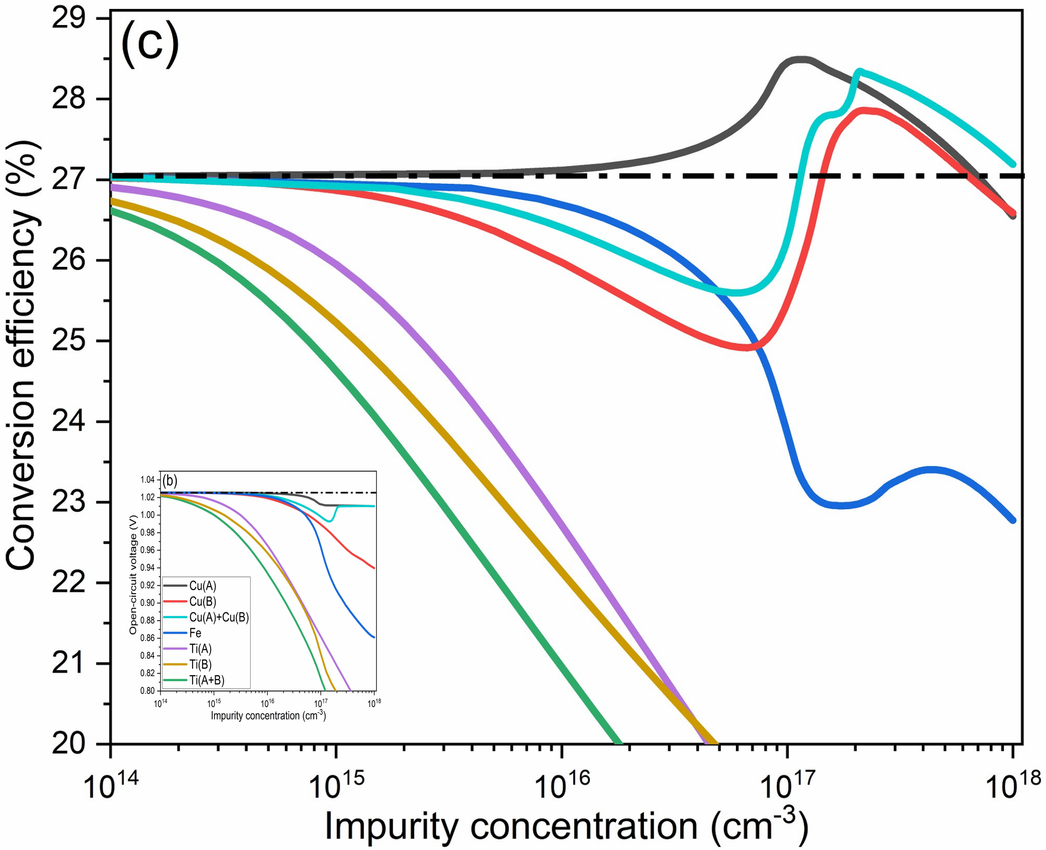


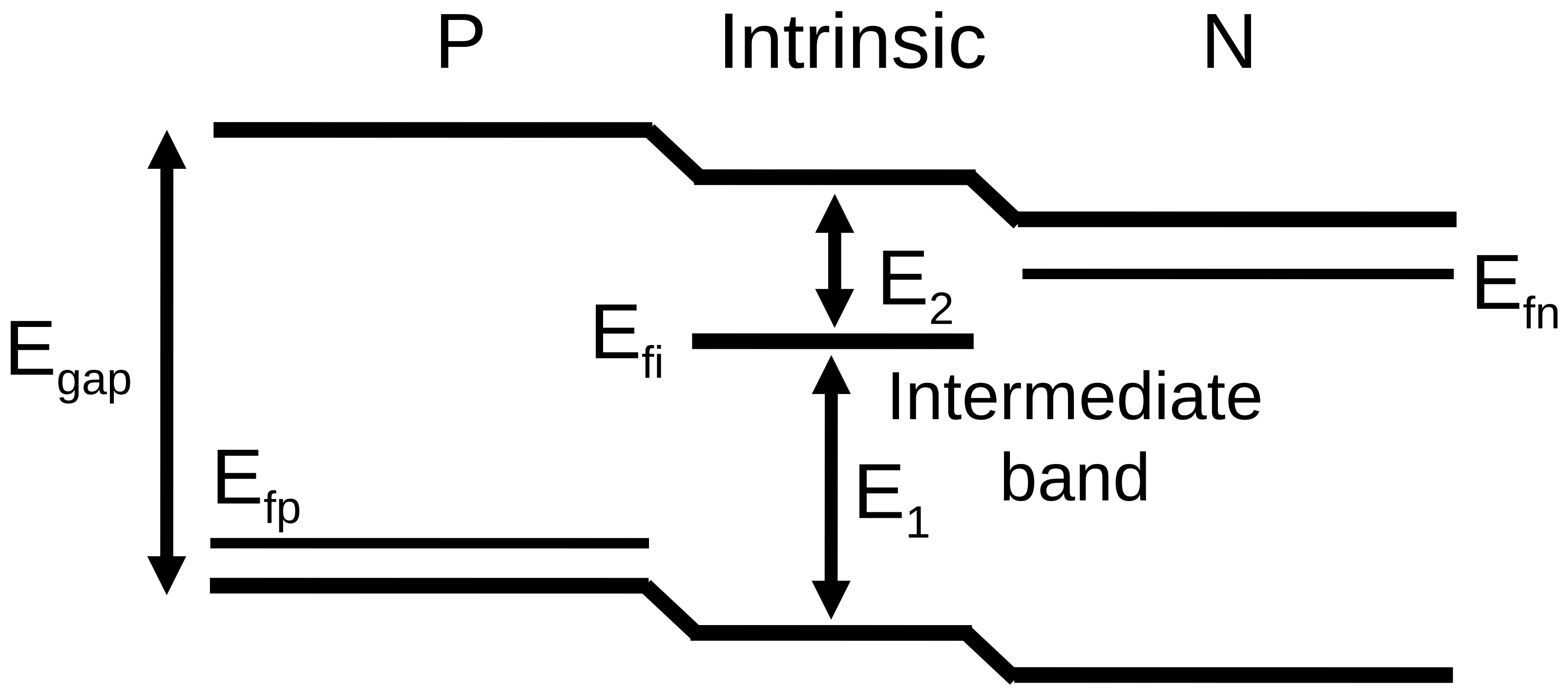

- $p^+/n/n^+$ layer structure
- Impurities in middle layer.

- Electron-capture cross sections:
- Ti ≈ $10^{-15}$ cm²
- Fe ≈ $10^{-19}$ cm²
- Cu ≈ $10^{-20}$ cm²

# GaAs-based impurity solar cell simulations

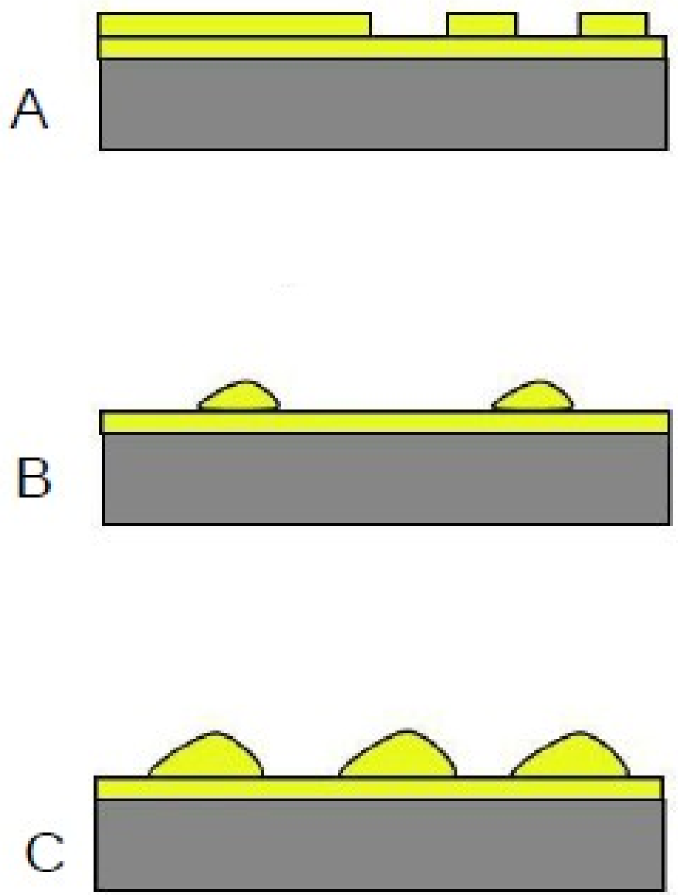


# Intermediate band solar cell



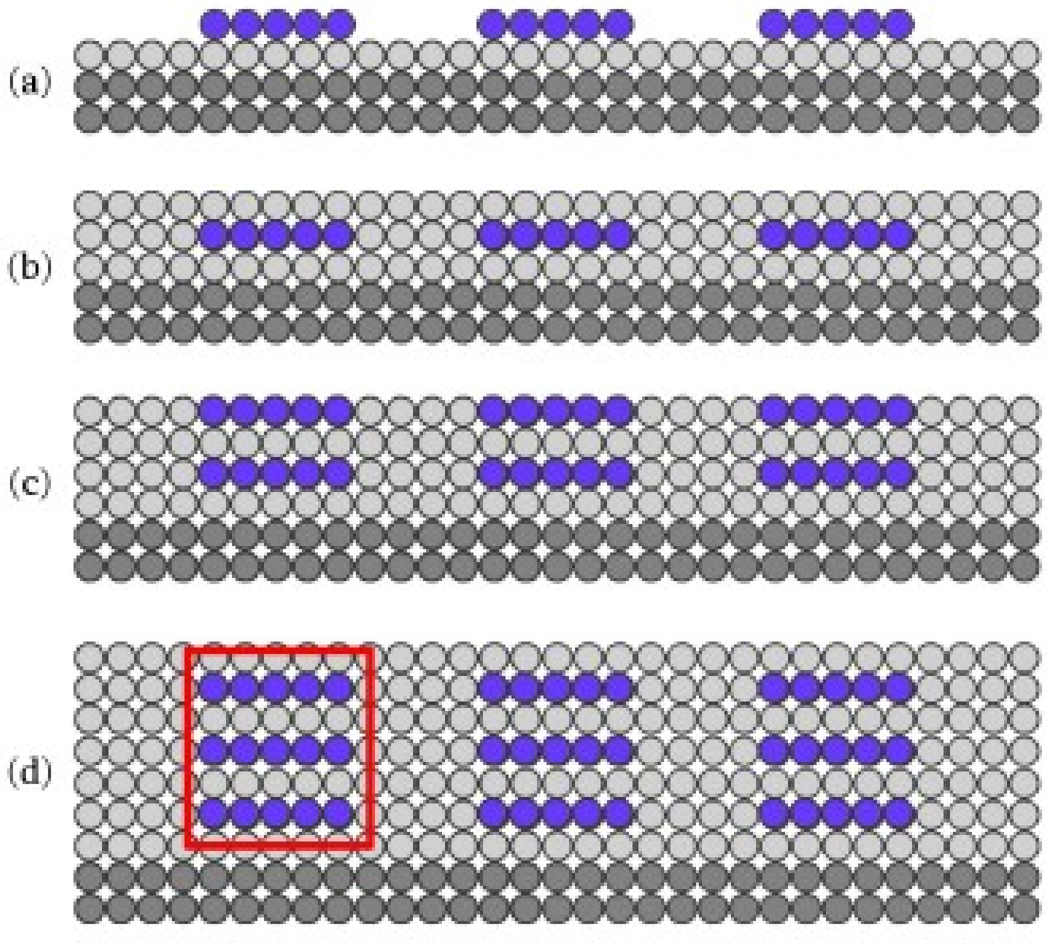

- Presence of an intermediate band in the bandgap.
- Intermediate band does not reach the contacts (carrier must be excited before collection).
- Null density of states in between bands (quase-Fermi level splitting).

# Stranski-krastanov quantum dots




- Common framework: InAs stranski-krastanov quantum dots in GaAs matrix.
- Strain is unavoidable → increase in recombination.
- Size and bound-state energy are not controllable parameters.

# Submonolayer quantum dots




**Technique**

1. Less than 1 monolayer of InAs is deposited.

2. A few monolayers of GaAs are deposited.

3. Repeat steps (a) and (b).

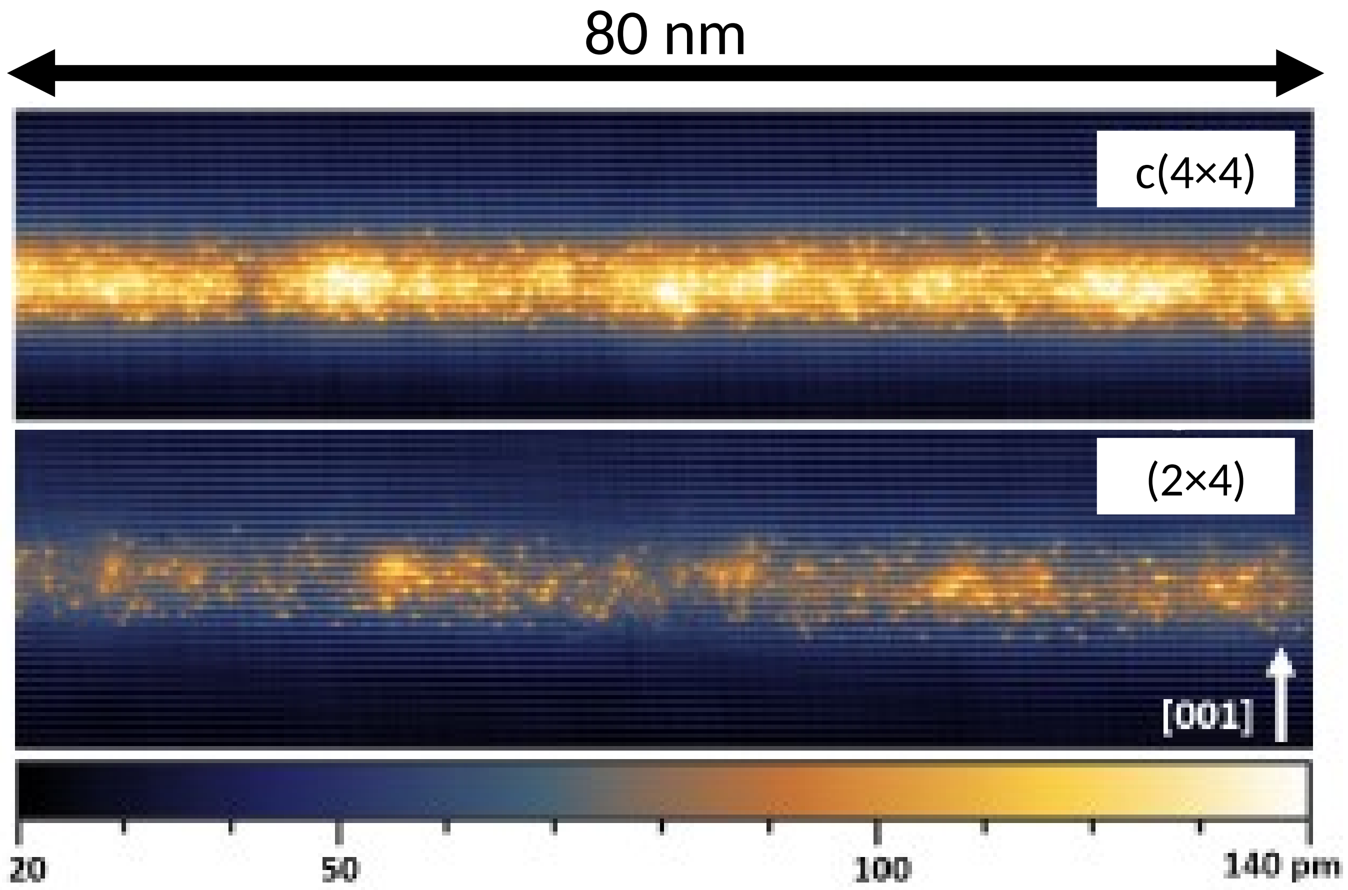
**A priori advantages**

1. Does require as much strain.

2. Adjustable size.

3. Areal density > $10^{12}$ $cm^2$

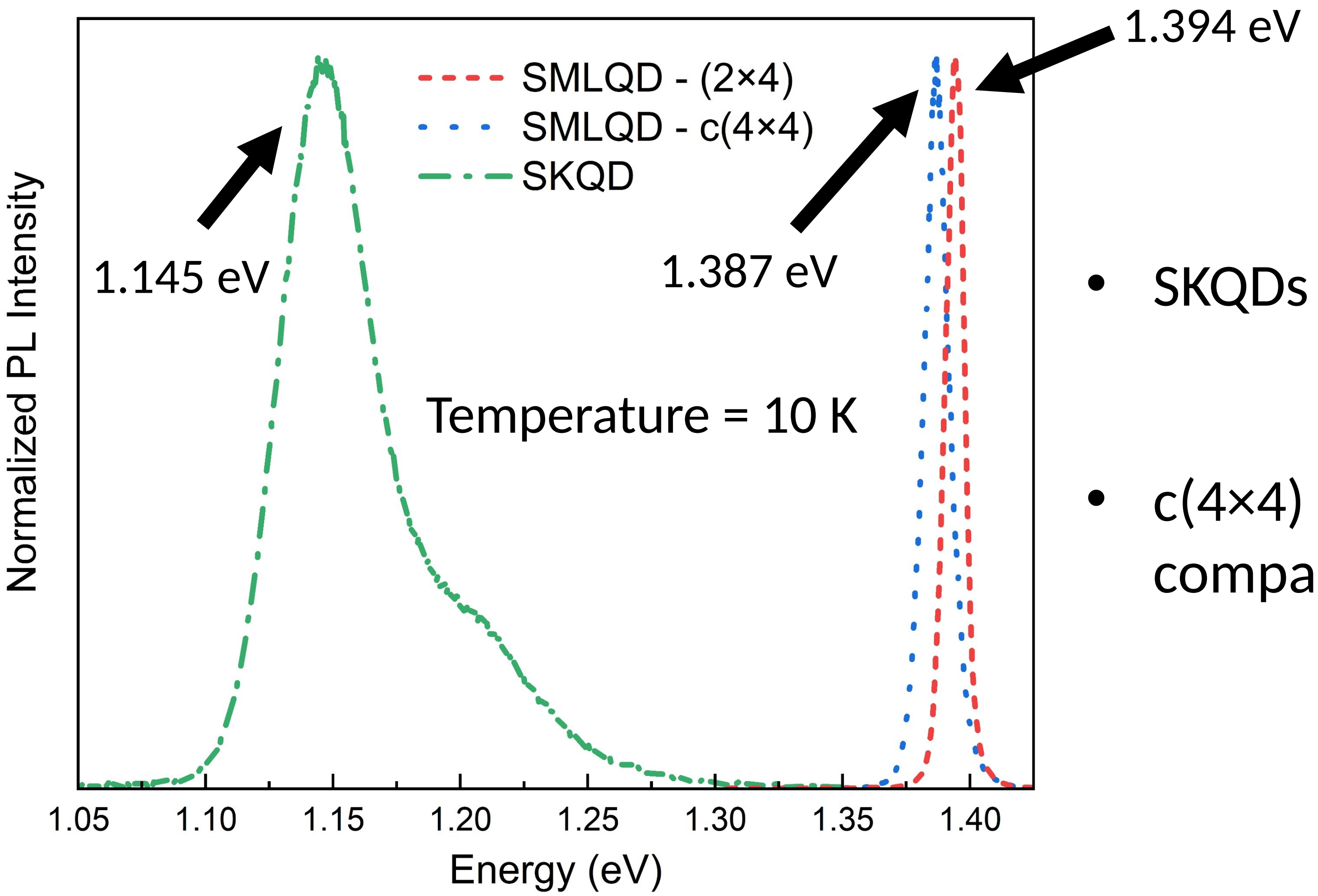
# Morphology – Cross-sectional scanning tunneling microscopy




- Segregation and low strain field → SMLQDs are diluted in a well.
- Much smaller than SKQDs.
- c(4×4) surface reconstruction leads to clusters with higher In concentration relative to (2×4).

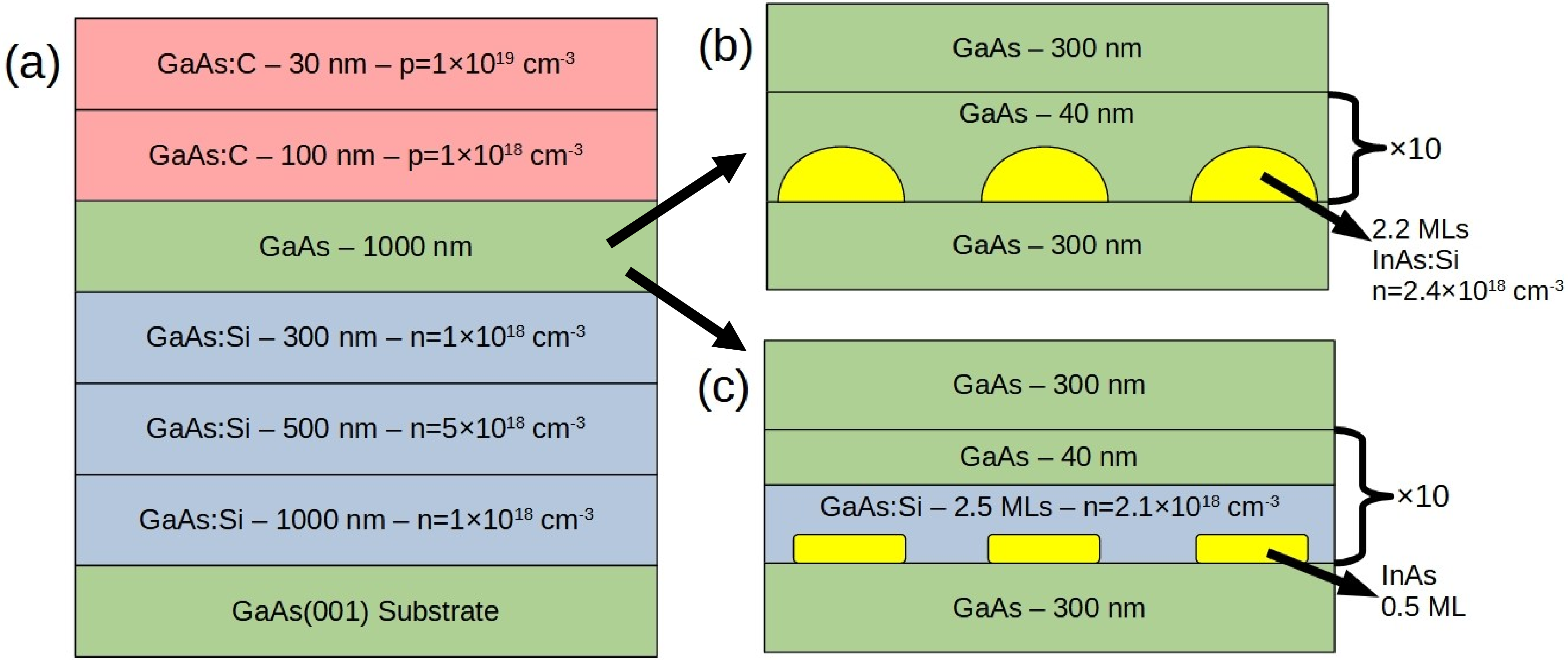
R. S. R. Gajjela, A. L. Hendriks, A. Alzeidan, T. F. Cantalice, A. A. Quivy, and P. M. Koenraad, Phys. Rev. Mater. 4(11), 114601 (2020). DOI: 10.1103/PhysRevMaterials.4.114601

# Energy level – Photoluminescence

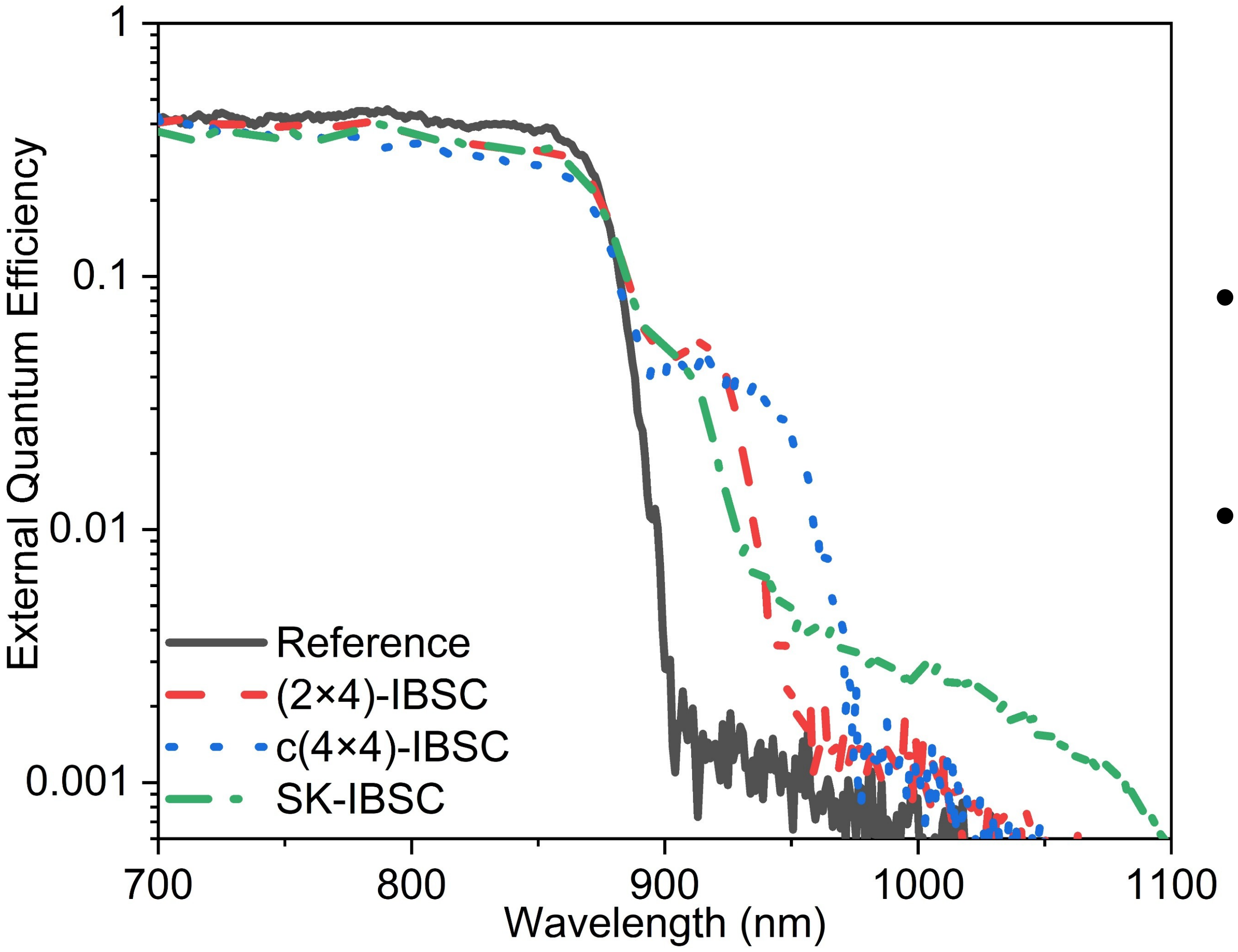



- SKQDs have a much higher In concentration.
- c(4×4) ground state has lower energy compared with (2×4).

# Solar cells grown by molecular beam epitaxy

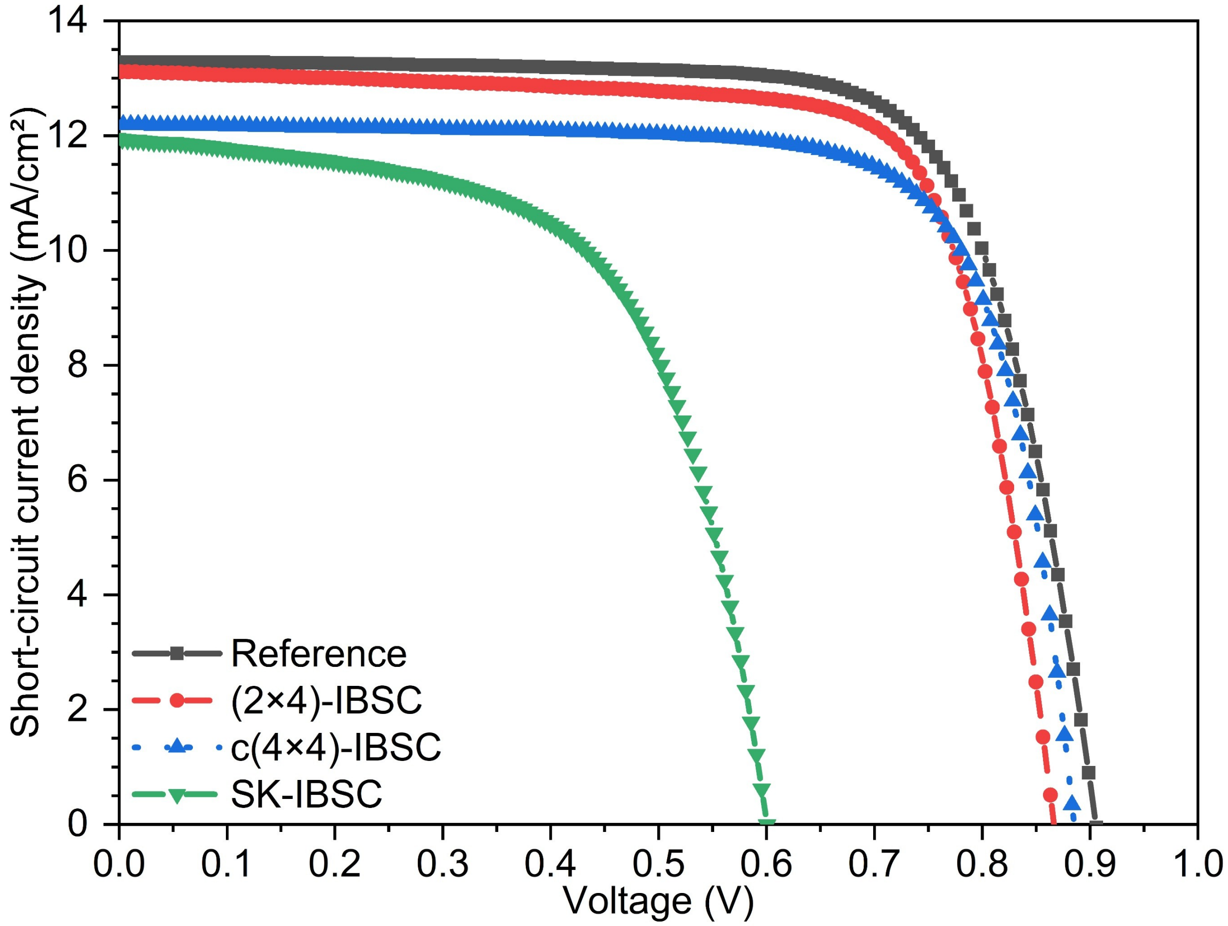


# External Quantum Efficiency




- Ranges are compatible with PL.
- SKQD has the lowest integrated EQE despite having a higher range.

# Illuminated I-V Curves




- SKQDs → much lower open-circuit voltage.
- SMLQD-IBSCs and Reference are similar.
- c(4×4)-IBSC has lower short-circuit current and higher open-circuit voltage than (2×4) → better confinement hypothesis.

# Take-home messages

- GaAs-based impurity solar cells should be further investigated, especially experimentally.
- SMLQDs lead to less carrier recombination and better performance compared with SKQDs.
- We have evidence of better carrier confinement when c(4×4) surface reconstruction is used.
- Further optimization of SMLQDs should be pursued. High-efficiency devices might be viable.

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