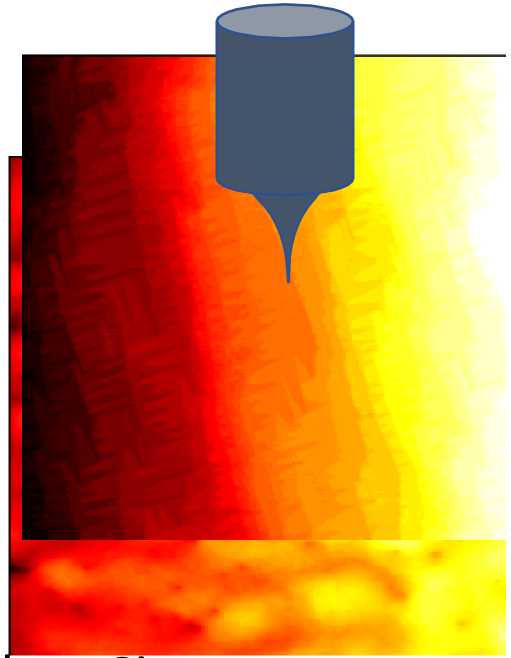
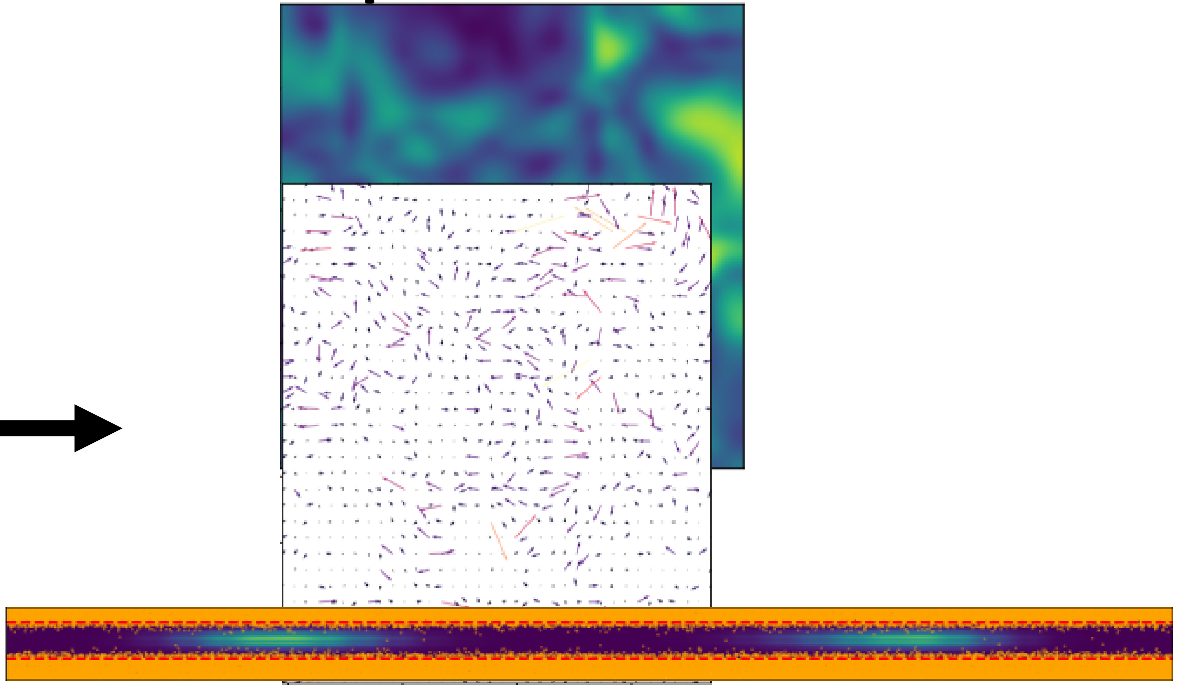
SAND2022-9604C

Scanning tunneling microscopy-informed simulation of valley physics in single and double quantum dots





Project: Silver City

PI: Toby Jacobson

Quantum Computing Program Review, July 2022

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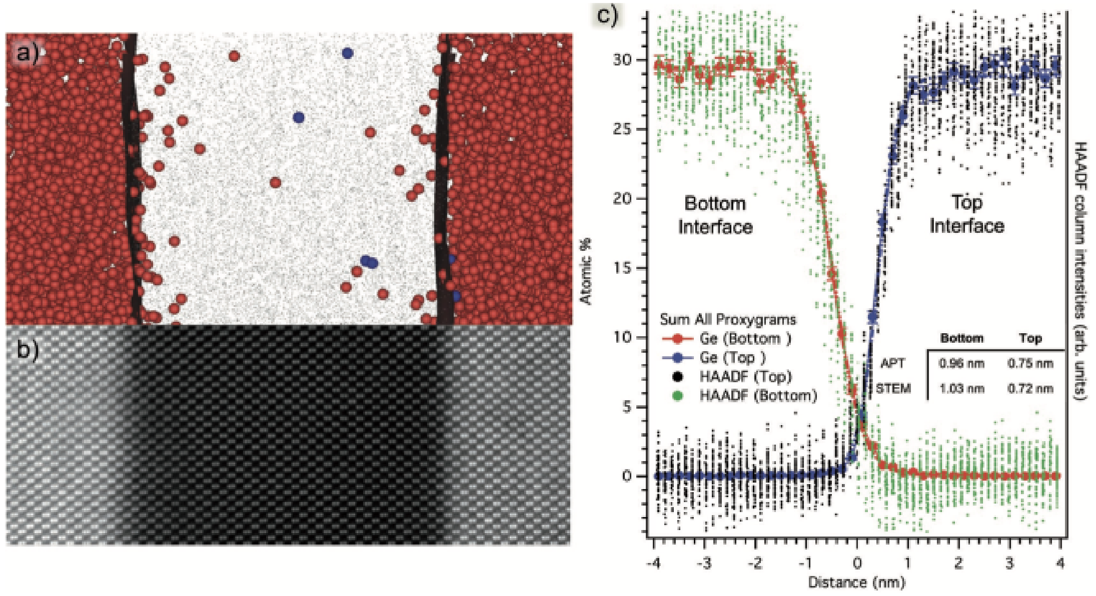
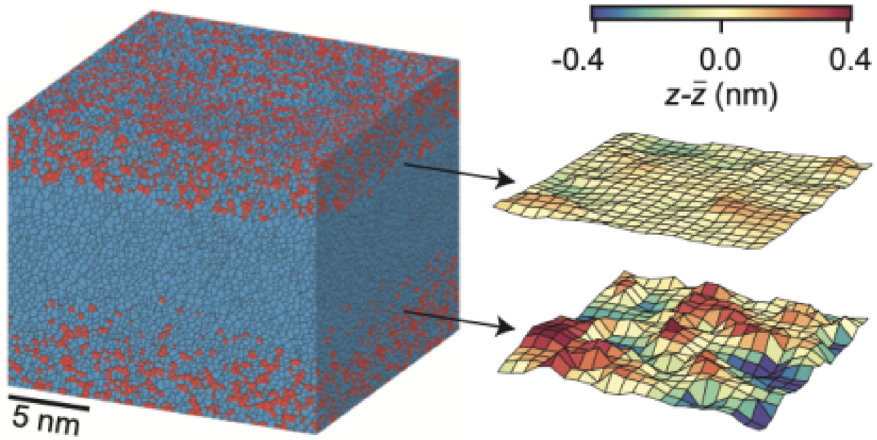
Center for Computing Research

Motivation

There's been much work recently to characterize SiGe/Si/SiGe wells, e.g.



[Dyck, et al. Adv. Mat. Interfaces 4, 1700622 (2017)]



[Wuetz, et al. arXiv:2112.09606]

Q: Given a realistic atomistic-level model for well structure, what are the consequences for quantum dot properties?

STM measurements of interface topography

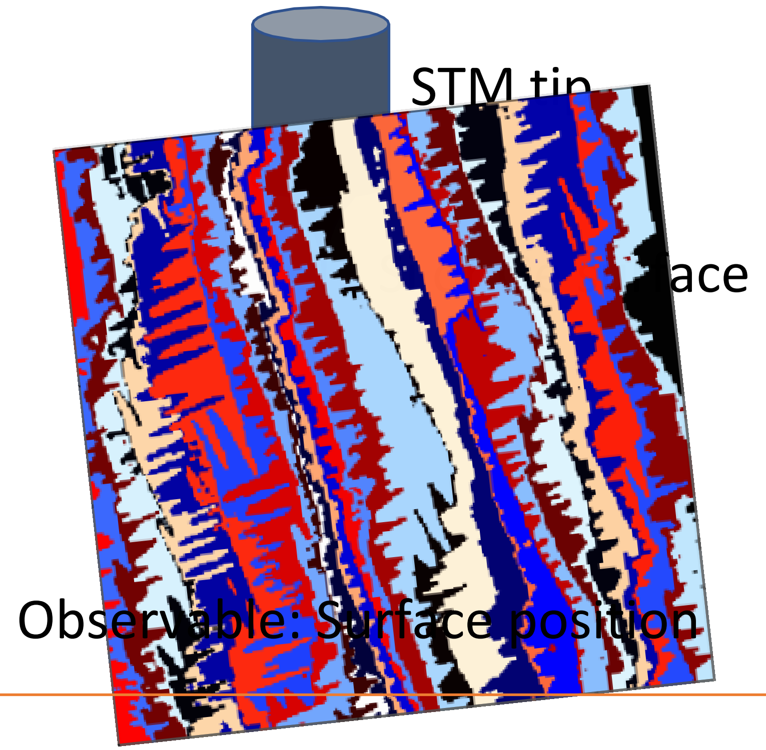
Scanning tunneling microscopy (STM) provides a means to characterize surface properties

Capability developed by Ezra Bussmann and collaborators (Sandia) under previous ARO/LPS-funded project

Procedure:

- Grow SiGe substrate
- Image surface of SiGe substrate w/ STM (lower interface)
- Continue growing Si well (molecular beam epitaxy)
- Image surface of Si well w/ STM (upper interface)

Cartoon of measurement



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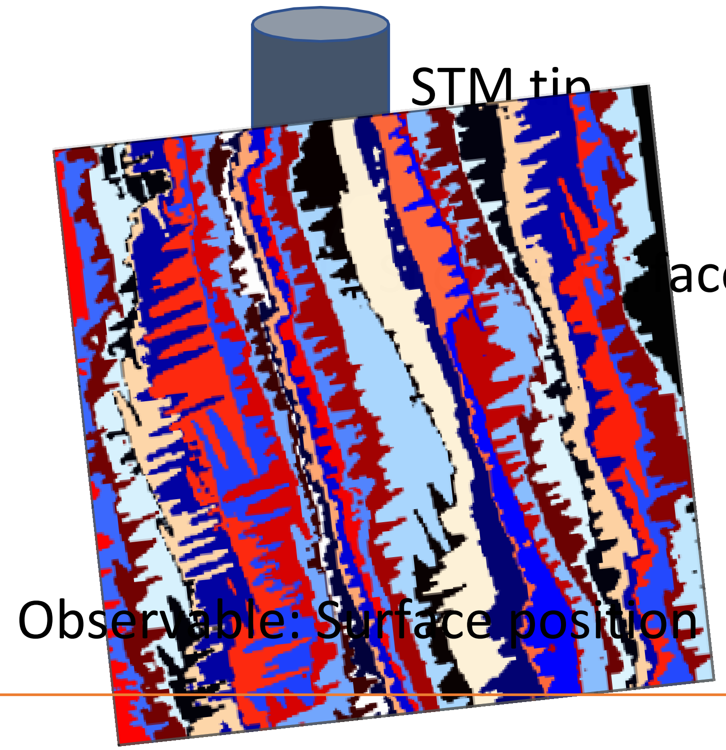
Result:

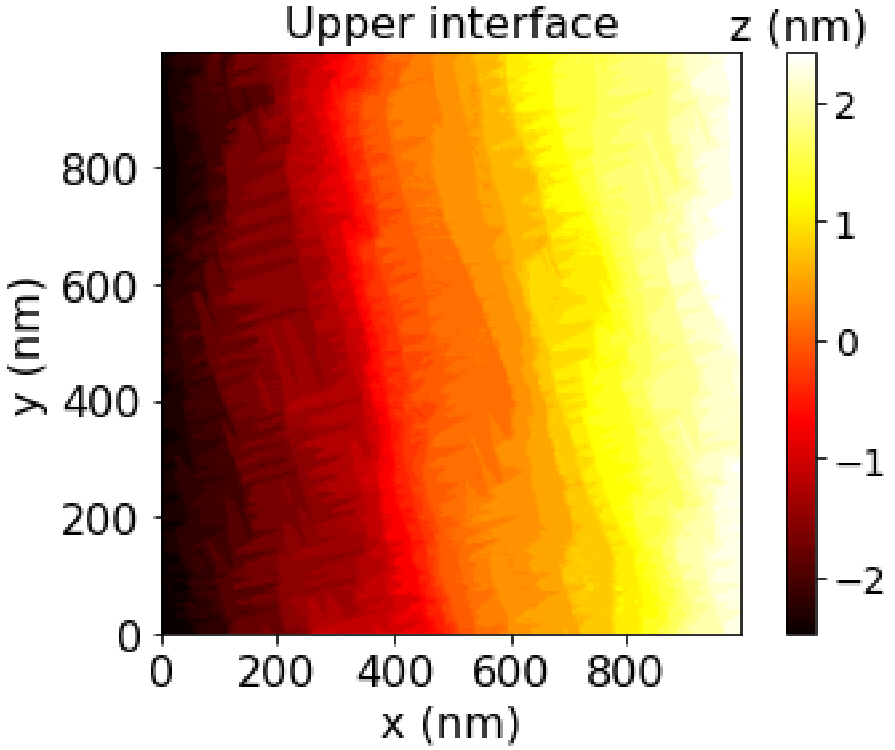
- Topography of both upper and lower interfaces of the Si well in the same device
- Use to generate an alloy disorder realization over a 1µm x 1µm x 15 nm volume, assuming some interdiffusion length

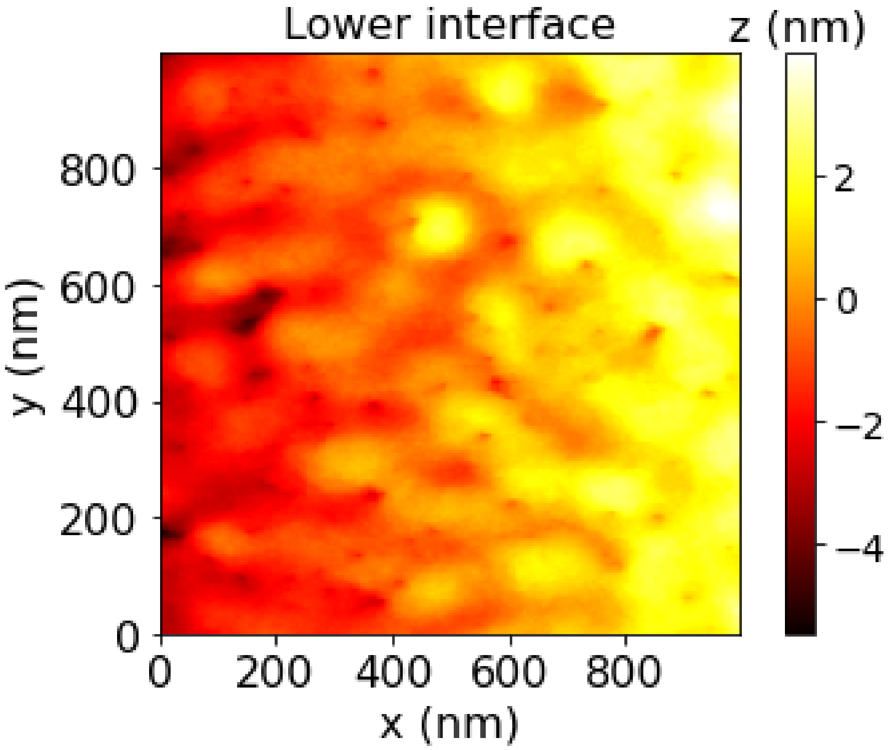
Cartoon of measurement



STM measurements of interface topography

Data courtesy Fabián Peña and Ezra Bussmann (SNL)





STM measurements of interface topography

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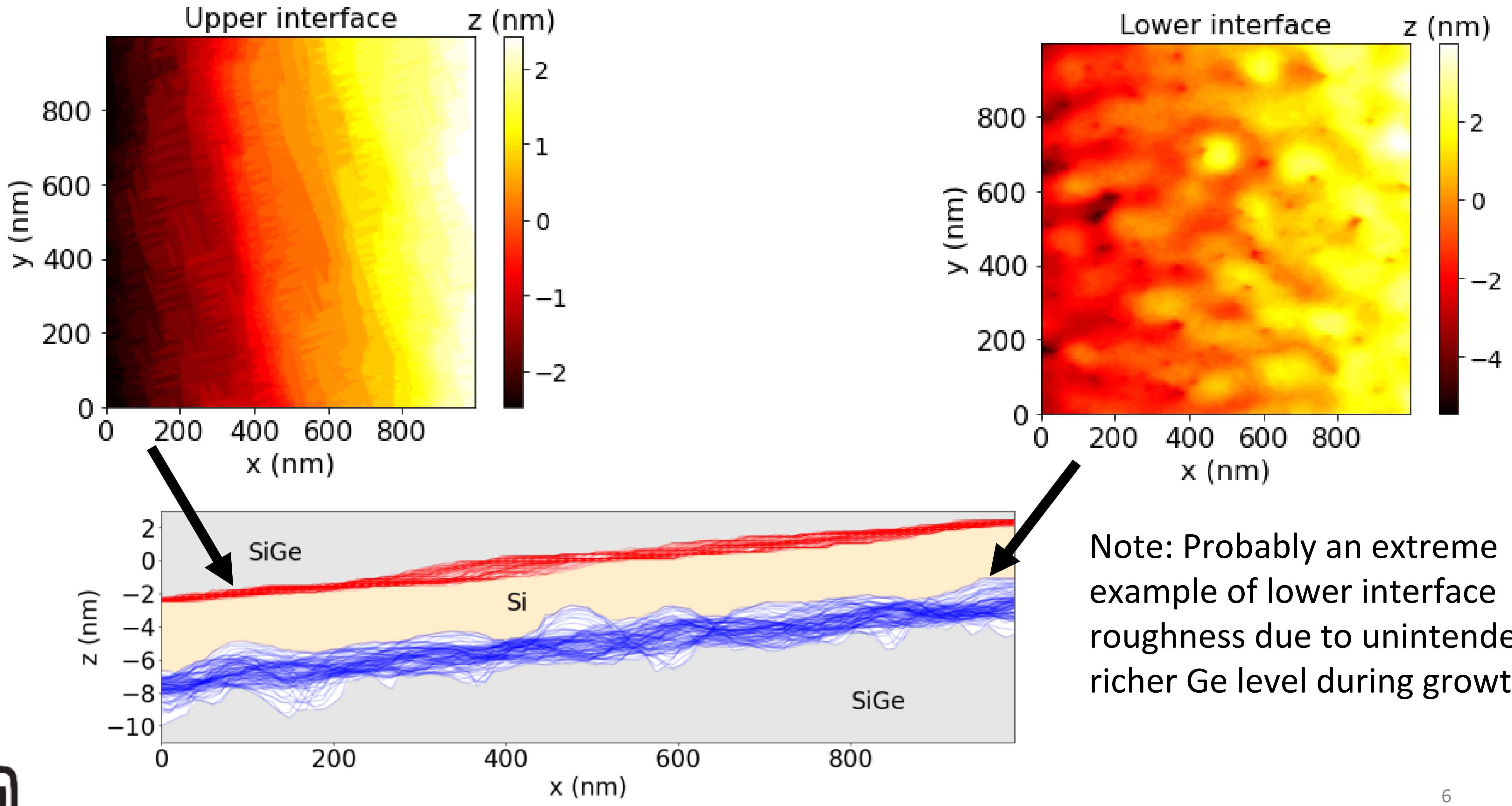


Note: Probably an extreme example of lower interface roughness due to unintended richer Ge level during growth

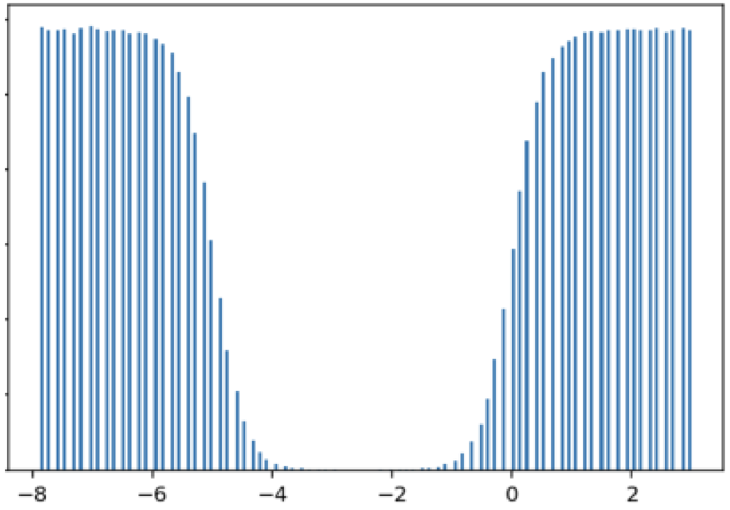
Atomistic disorder model

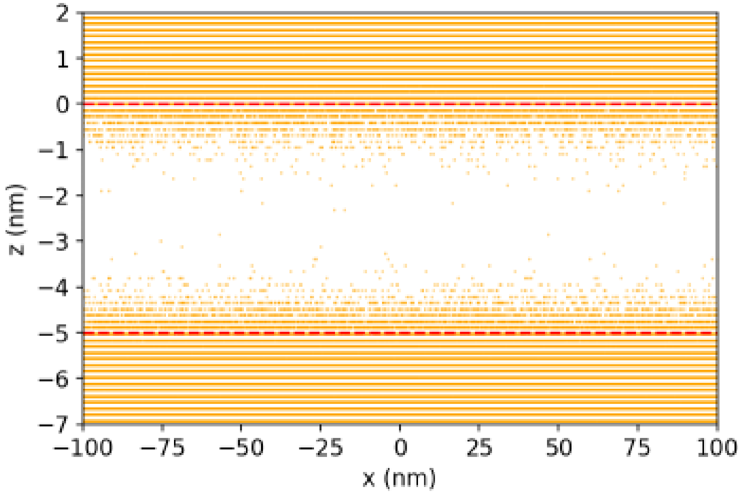
- Use STM data or idealized model ("flat interface") to define the interface locations in (x,y) plane
- For each interface, define a sigmoidal Ge concentration along *z*-axis, referenced to local interface location $z_{\text{upper}}(x,y), z_{\text{lower}}(x,y)$
- Generate an alloy realization on diamond lattice for all atoms (~10^9 atoms) and down-select based on simulation volume
- Including both "step" structure and interdiffusion

- In the following, assuming 4τ=1 nm based on TEM measurements of 25 nm thin lamellae [Bussmann]
  - Consistent also with other APT and HAADF-STEM measurements:

  [Dyck, et al. Adv. Mat. Interfaces 4, 1700622 (2017)]
  [Wuetz, et al. arXiv:2112.09606]

Example Ge fraction histogram



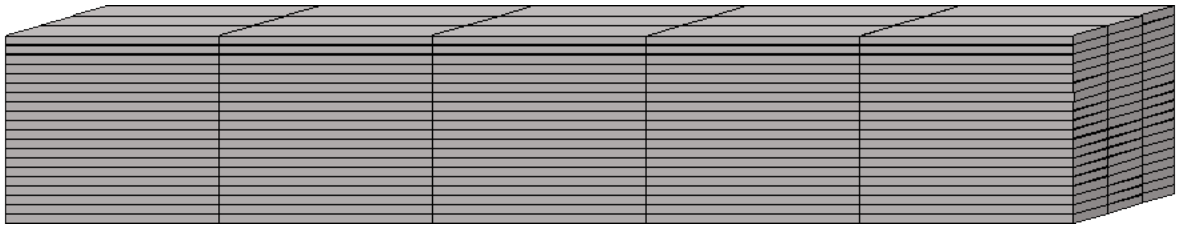


Sigmoidal interdiffusion distribution [Dyck, et al. (2017)]:

$$f(z) \propto 1/(1+e^{-z/\tau})$$

Model

- ***Mesh-based discretization***
  - Legendre polynomials on a hexahedral mesh (stack of bricks)
  - Taking up to 3rd order here (64-dim modal basis/mesh element)
  - Discontinuous Galerkin formulation in *Laconic* code developed at Sandia
  - High-throughput simulations feasible: <1 hr/eigensolve on single core



Mesh highly refined along *z*-axis to resolve wavefunction tails near interfaces

Model

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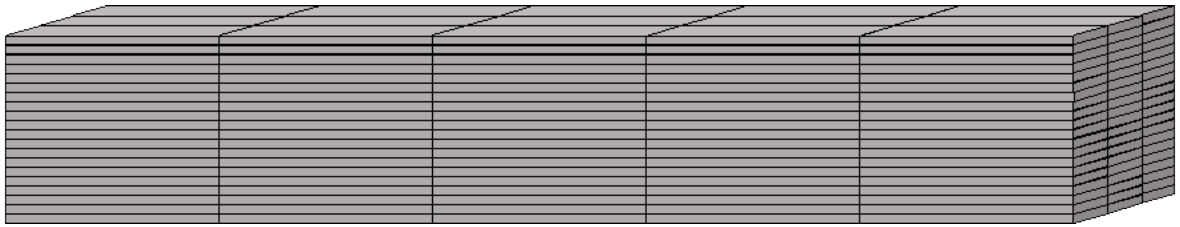
  - Discontinuous Galerkin formulation in *Laconic* code developed at Sandia
  - High-throughput simulations feasible: <1 hr/eigensolve on single core
- ***Valley-orbit coupling:***
  - Shindo-Nara equations [Shindo & Nara (1976)] for multi-valley EMT
  - Plane wave representation of Bloch functions from DFT
  - Atom-by-atom model for valley-orbit coupling: Each Ge atom contributes a ***localized*** repulsive potential scaled to agree with concentration-dependent Si → SiGe CB offset



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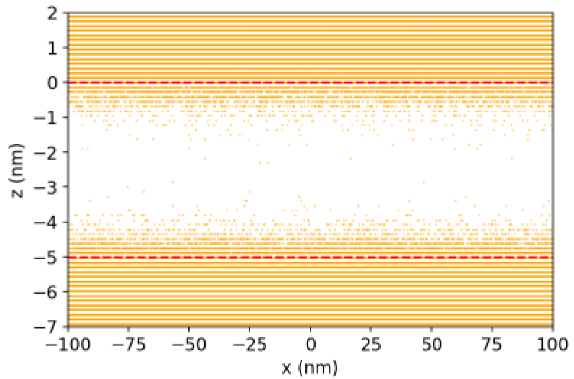


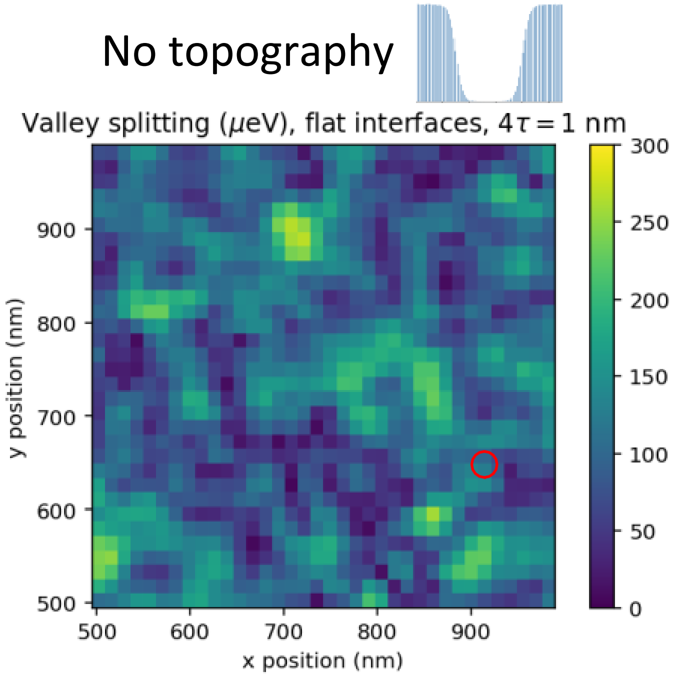
$$V_{\mathrm{Ge},i}(\mathbf{r}) = \alpha_{\mathrm{Ge}}\delta^{(3)}(\mathbf{r}-\mathbf{r}_i), \quad \alpha_{\mathrm{Ge}} = 12\ \mathrm{meV\ nm}^3$$

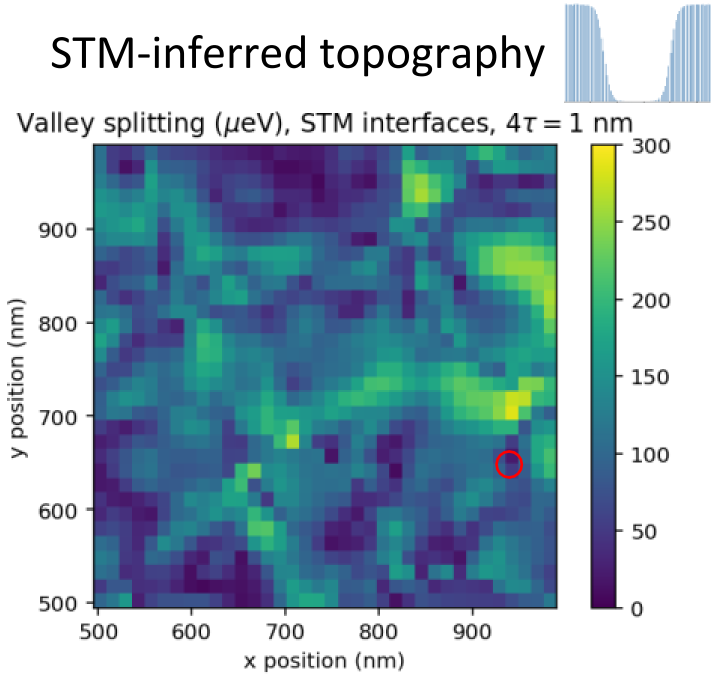
$$\langle \mathbf{r}|u_{\pm z}\rangle = \sum_{\mathbf{G}} c_{\mathbf{G},\pm z} e^{i\mathbf{G}\cdot\mathbf{r}}$$

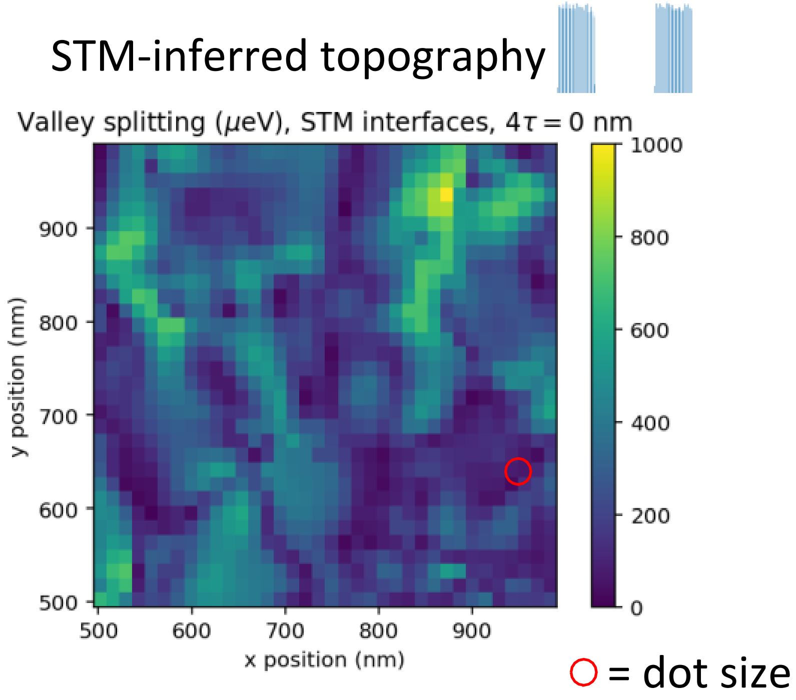
$$\langle u_{\pm z}|\delta^{(3)}(\mathbf{r}-\mathbf{r}_i)|u_{\pm z}\rangle \approx 1$$

$$\langle u_{\pm z}|\delta^{(3)}(\mathbf{r}-\mathbf{r}_i)|u_{\mp z}\rangle \approx 1$$

Single quantum dot rastered across the surface: Valley splitting

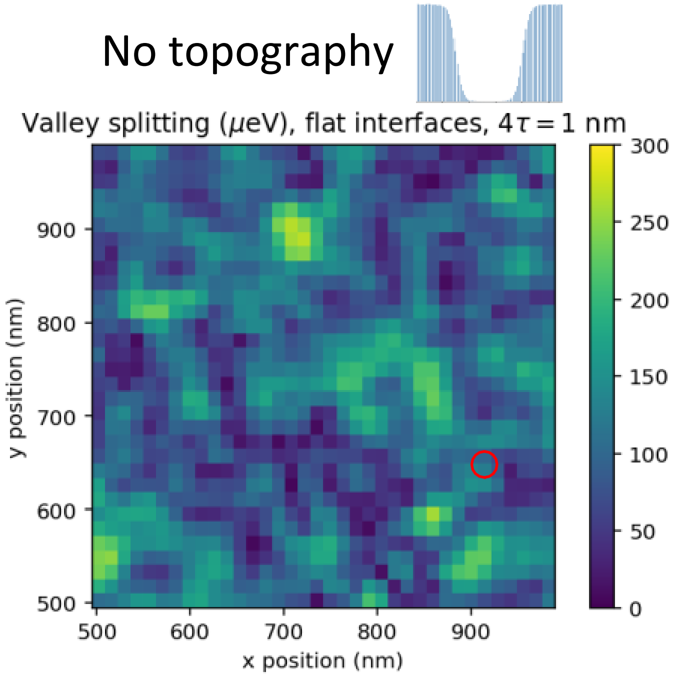


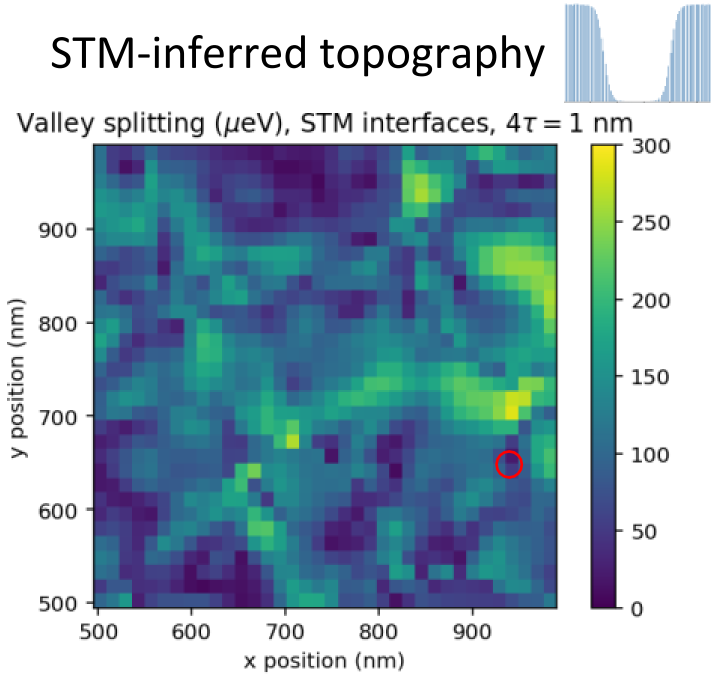


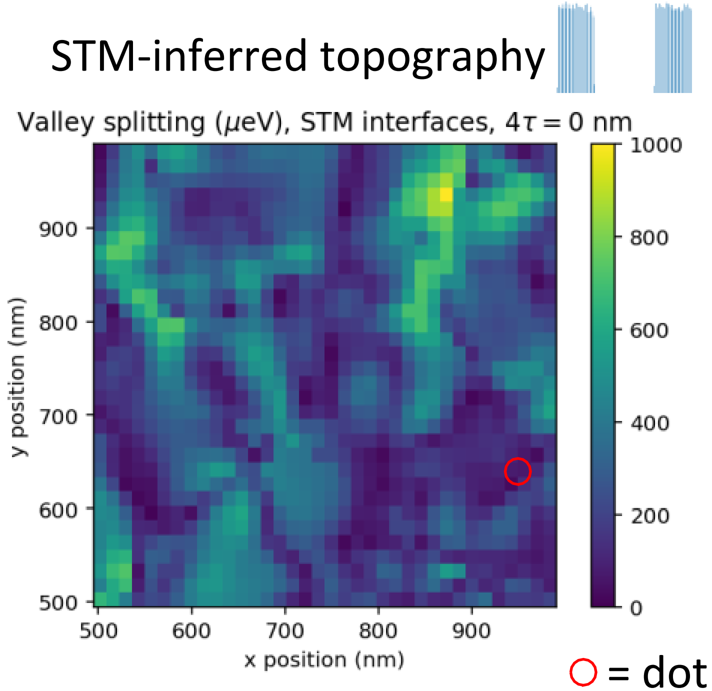


- 1.5 meV symmetric harmonic *x*-*y* confinement

Single quantum dot rastered across the surface: Valley splitting

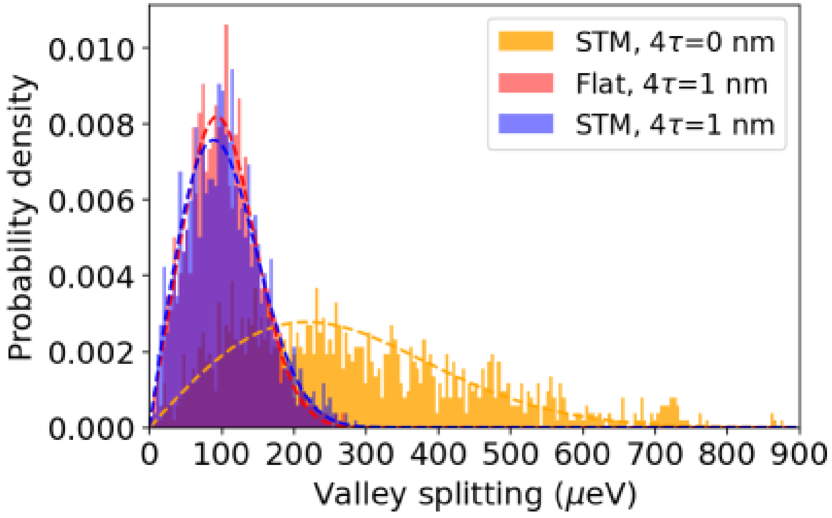


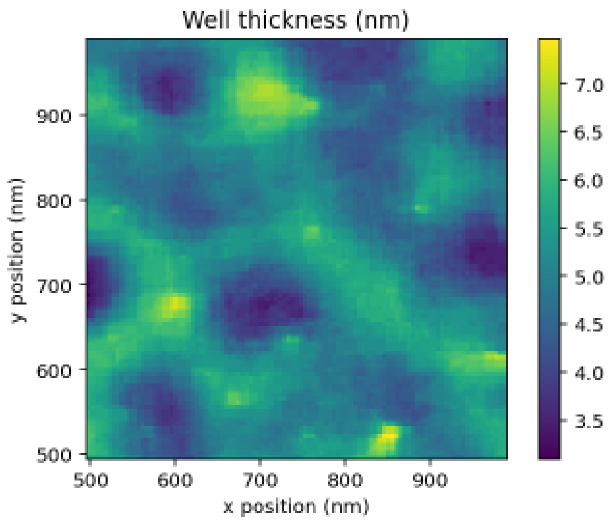




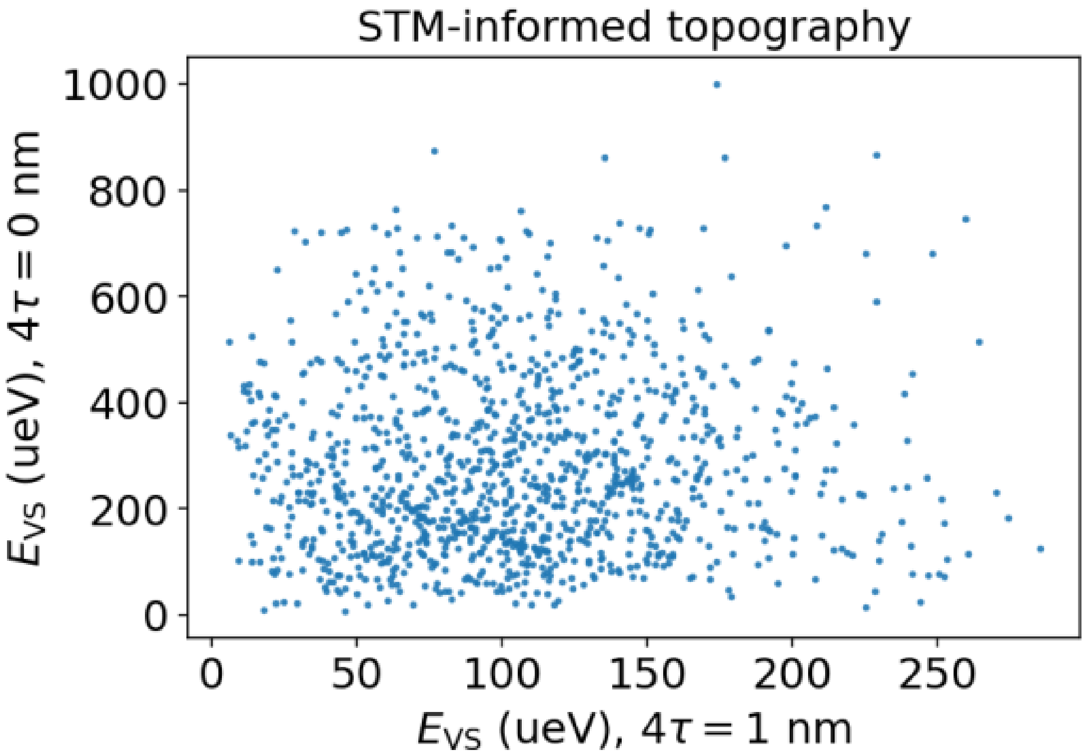
○ = dot size

- 1.5 meV symmetric harmonic *x*-*y* confinement
- Decent fit to Rice distribution for valley splitting [Wuetz, et al. (2021)]
- Interdiffusion length 4*τ* has a strong effect on valley splitting
- Atomic steps/topography appear to be less important than interdiffusion





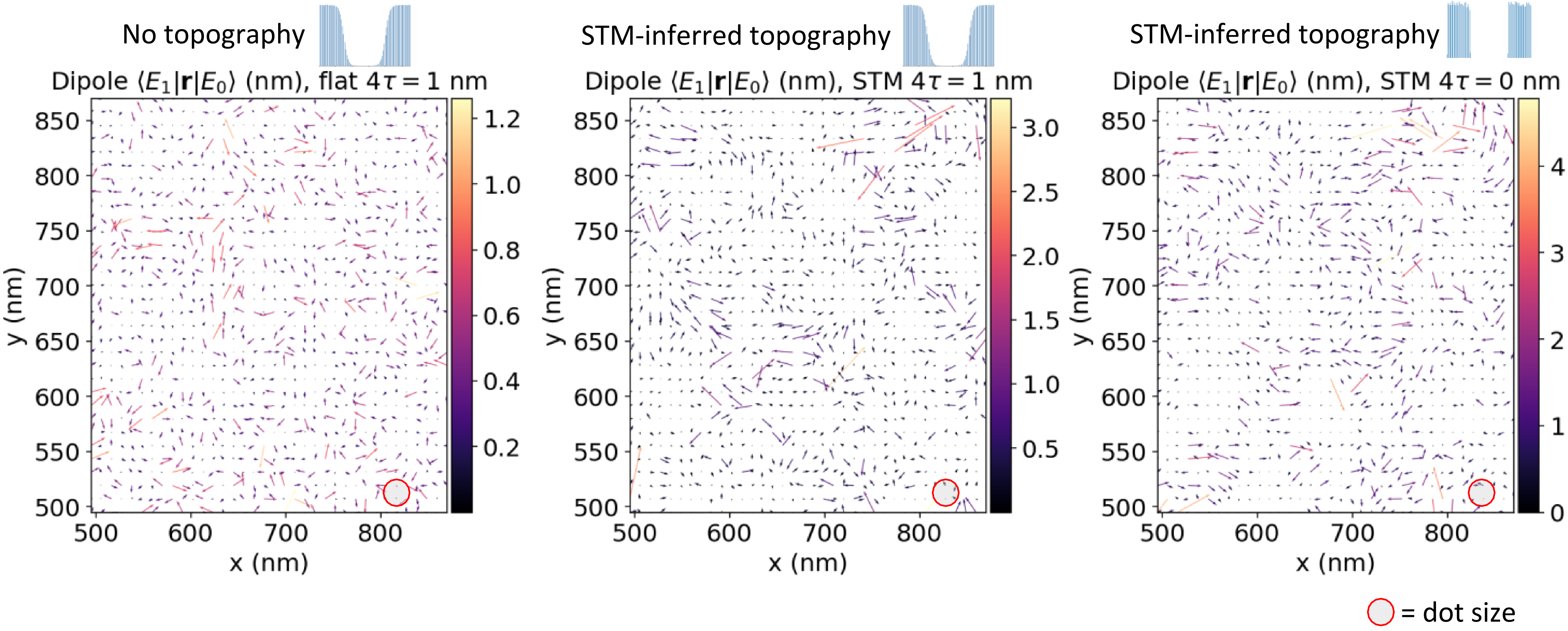
Single quantum dot rastered across the surface: Valley splitting



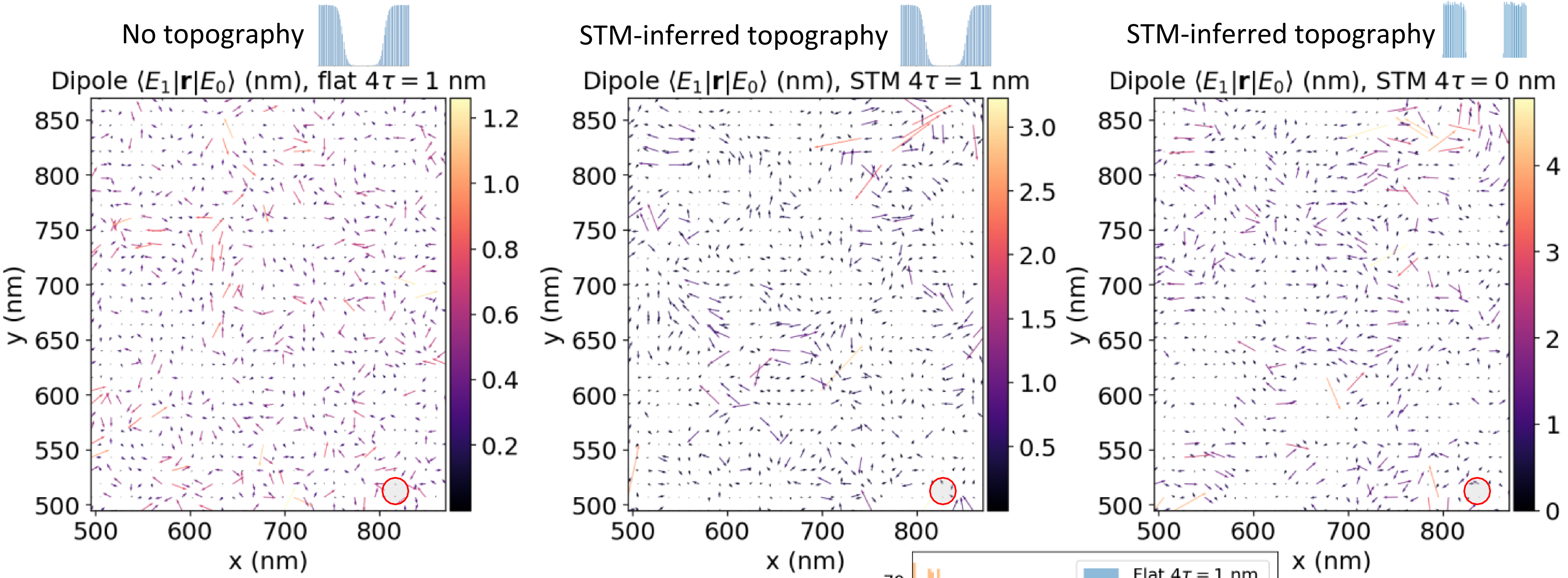
Each point: Same *x-y* confinement coordinate

- Valley splitting uncorrelated between different interdiffusion lengths 4τ for same interface topography
- Interdiffusion appears to be the dominant driver of valley splitting

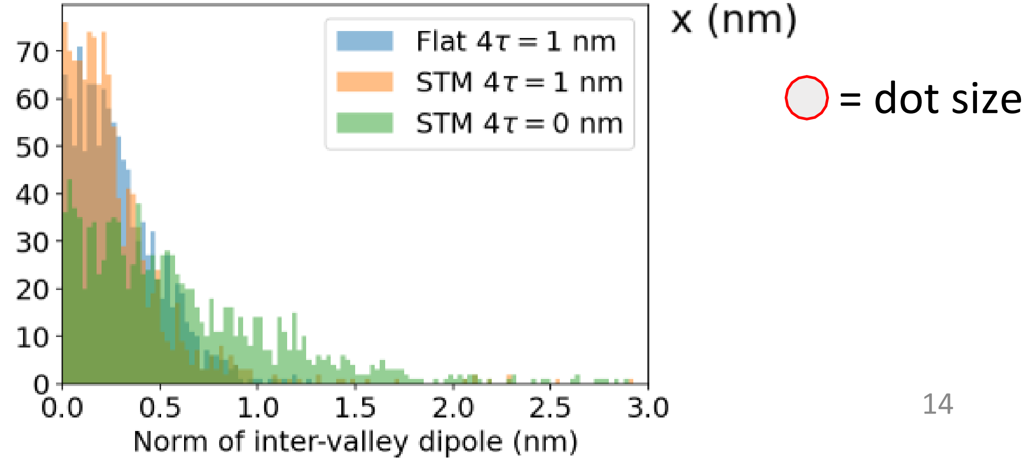
Single quantum dot rastered across the surface: Inter-valley dipole



Single quantum dot rastered across the surface: Inter-valley dipole

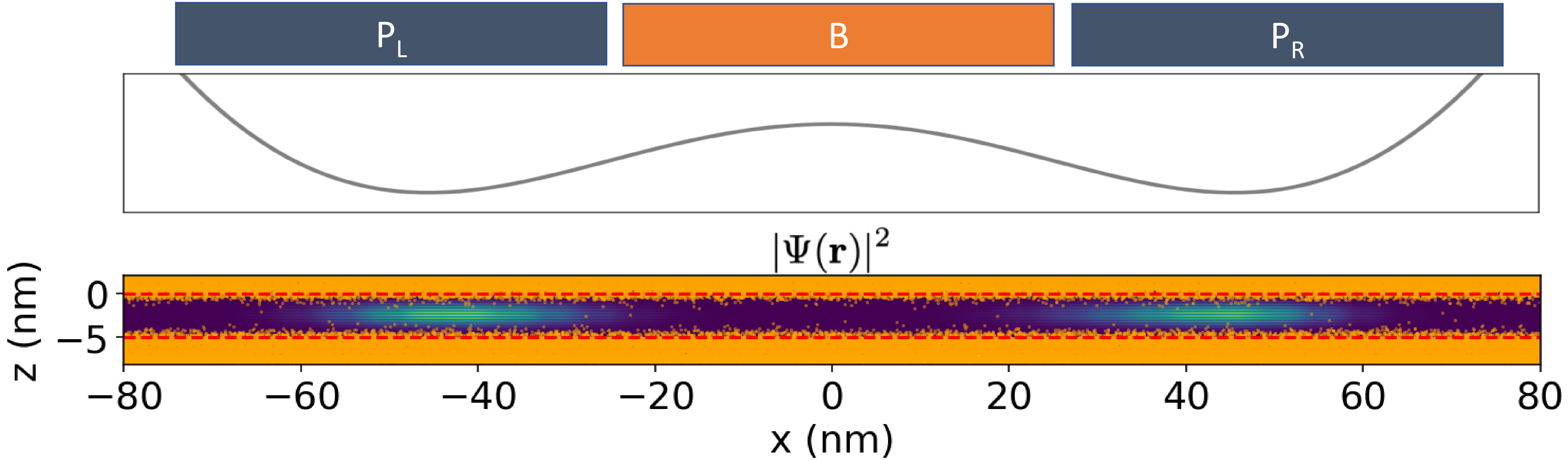


- Inter-valley dipole should relate to spin-orbit coupling properties, e.g. spin-valley coupling [Yang, et al. Nat. Comm. 4, 2069 (2013)]
- Generally larger dipole in presence of crisp interface topography



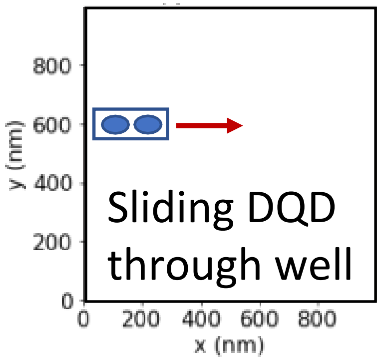
Double quantum dot

- Assuming "benchmark" double well potential of [Anderson, et al. arXiv:2203.00082]
- 5 nm well
- Interface topographies: flat or STM-inferred
- Interdiffusion length, 4τ: 0 or 1 nm



Orange dots: Ge atoms within ±5 nm of x-z cut plane

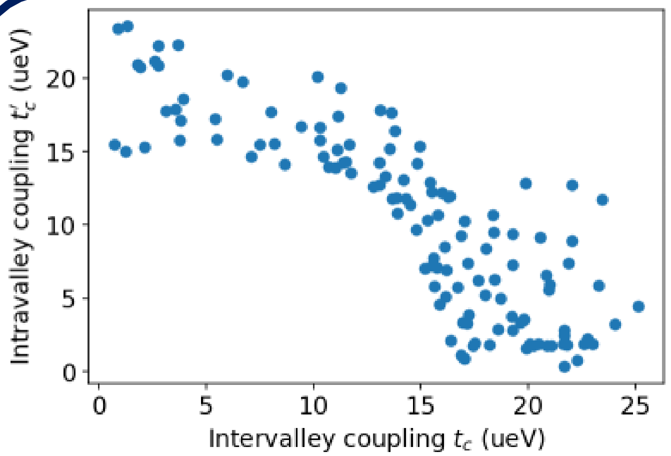
Double quantum dot: Flat interfaces



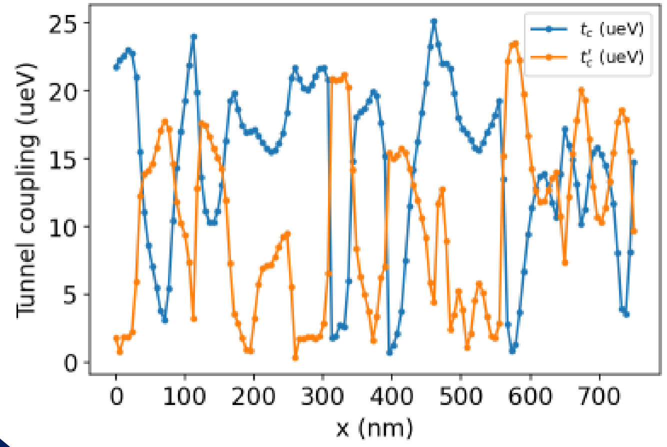
- Compute position dipole and infer four-level Hamiltonian
- Fits nicely to the 4-level double dot model of [Borjans, et al. PRX Quantum 2, 020309 (2021)]

$$H = \begin{pmatrix} \frac{\epsilon}{2} & 0 & t_c & t'_c \\ 0 & \frac{\epsilon}{2} + E_{\mathrm{VS,L}} & t'_c & t_c \\ t_c^* & t_c'^* & -\frac{\epsilon}{2} & 0 \\ t_c'^* & t_c^* & 0 & -\frac{\epsilon}{2} + E_{\mathrm{VS,R}} \end{pmatrix}$$

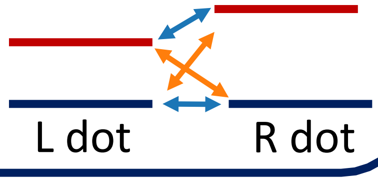
- Extract:
  - Valley splittings $E_{\mathrm{VS,L}}$, $E_{\mathrm{VS,R}}$
  - Intra-/inter-valley tunnel couplings t_c, t'_c
  - Detuning offset ϵ_0 due to alloy disorder

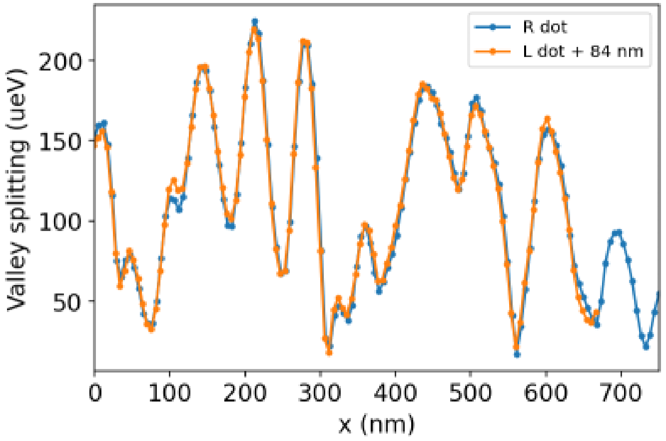


Intra-/inter-valley tunnel couplings are anticorrelated, as expected



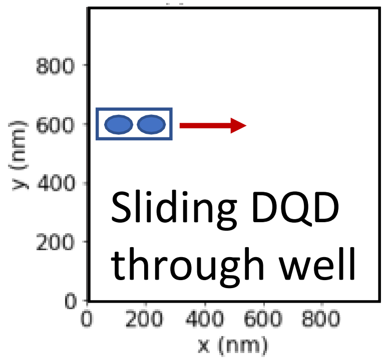
t_c = intravalley
t'_c = intervalley



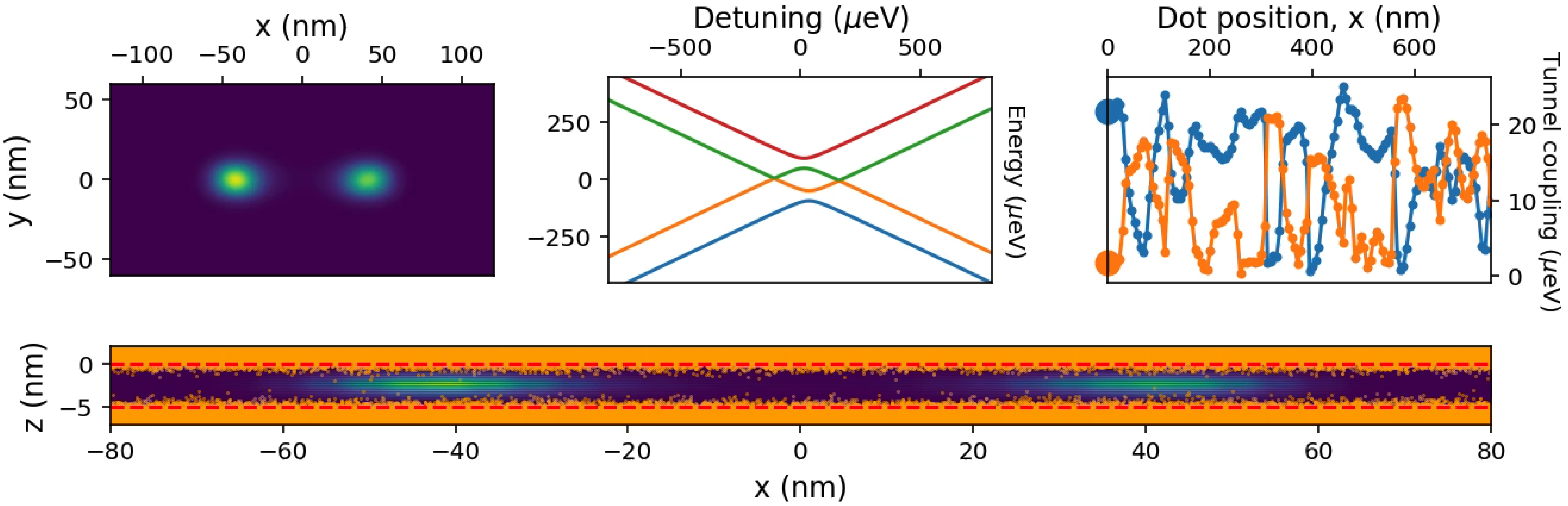


E_{VS} consistent with single-dot behavior, as expected

Double quantum dot: Flat interfaces



t_c = intra-valley tunnel coupling
t'_c = inter-valley tunnel coupling



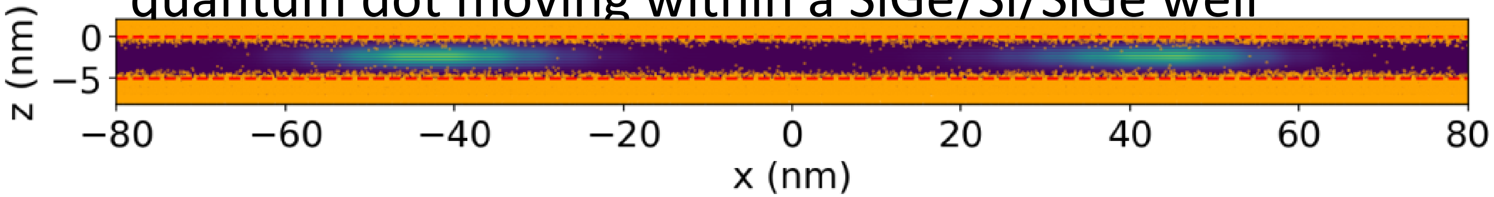
For STM-informed interfaces, alloy disorder-induced detuning variation is much more dramatic (approximately 10x)

Summary

- We've developed machinery for simulating large-scale atomistic alloy disorder within multi-valley effective mass theory based on information about interface topography
  - Able to use data from e.g. APT, STM characterization of atomic-scale disorder

- For significant interdiffusion between Si and SiGe layers, **valley splitting** and **inter-valley dipole** statistics primarily governed by diffusion rather than interface topography

- We've characterized inter- and intra-valley tunnel coupling variation for a double quantum dot moving within a SiGe/Si/SiGe well



Acknowledgements:

- Ezra Bussmann (Sandia)
- Fabián Peña (formerly at Sandia)
- Mitchell Brickson (UNM)
- Andrew Baczewski (Sandia)