

Enhanced diffusion at heterogeneous interfaces in Cu/AlN nano-multilayers

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Introduction

- The outflow of Cu in nano-confinement with AlN at strikingly low temperatures enables low-temperature joining in micro- and nano-electronics [1-6].

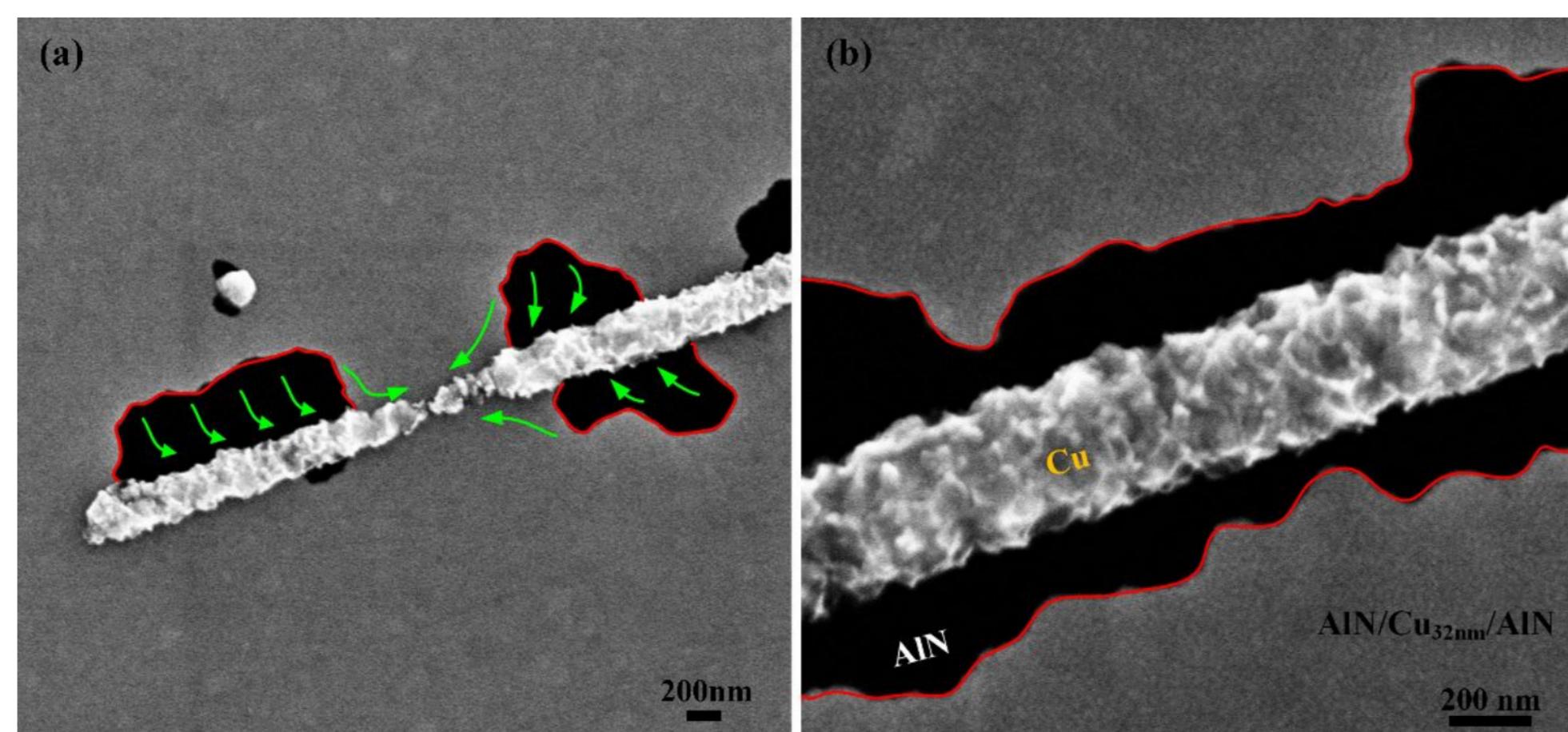


Figure 1: SEM of Cu outflow to the surface of AlN [6]

- The interface free volume promotes the formation of Frenkel pairs, which can enhance solid-state diffusion and interface premelting [7].
- The role of equilibrium vacancies in such processes has not been evaluated so far.
- Interfaces can enhance solid-state diffusion by lowering the vacancy formation or vacancy migration energies, which are analyzed in this work by using first-principles calculations.

Methods

- The bilayer supercell with Cu[111]/AlN[0001] interfaces is constructed in the *Cell/Match* code with 0.685% strain in Cu.

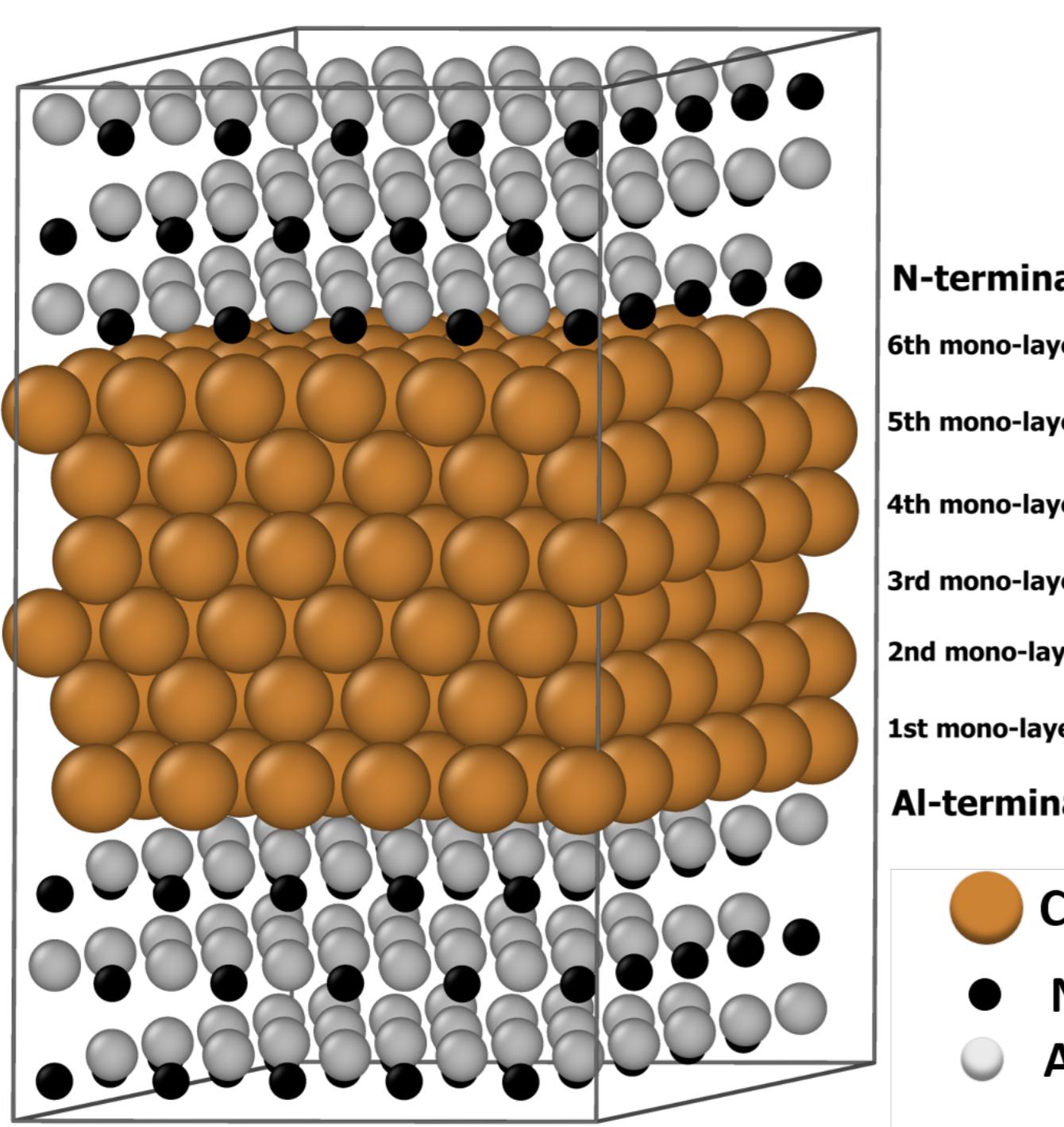


Figure 2: Initial configuration

- Ab initio* electronic-structure calculations, performed using *Quantum ESPRESSO* code with PBE exchange-correlation functional.
- Some of the Cu atoms exhibit polar-covalent bonds with N at the N-terminated interface.

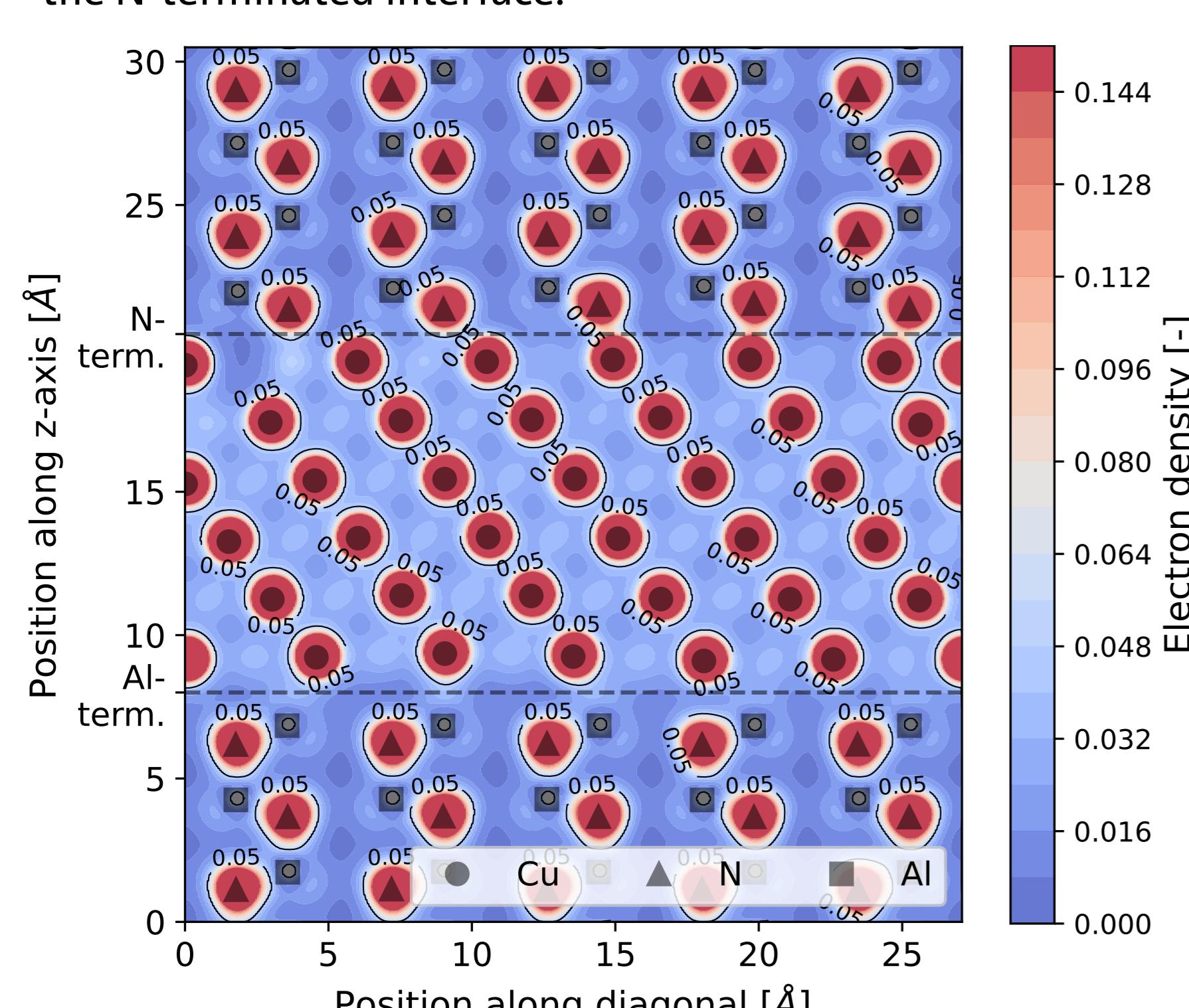


Figure 3: Electron density through the main diagonal.

- Metallic bonds are formed at the Al-terminated interface.

Vacancy Formation

- Vacancy formation energies near interfaces are generally lower than in the middle of the Cu layer.

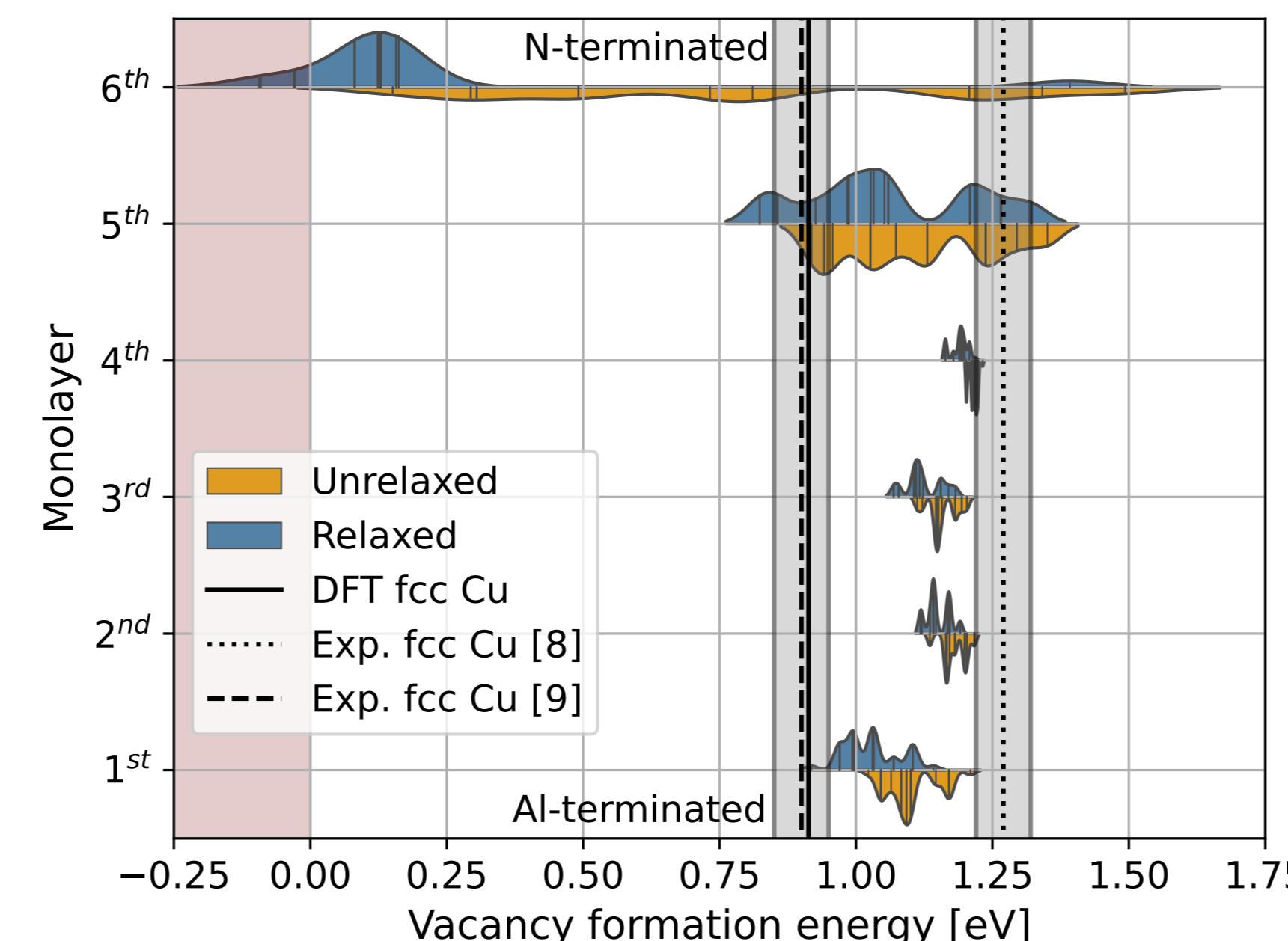


Figure 4: Distributions of the vacancy formation energies in Cu mono-layers before (orange) and after (blue) relaxation. Higher than the bulk Cu values in the middle layers is the result of the misfit strain. Experimental results from the literature [8,9] are displayed as well.

- Negative vacancy formation energies suggest that the N-terminated interface is unstable.
- Stabilization of the interface at 0 K requires the extraction of at least two Cu atoms.

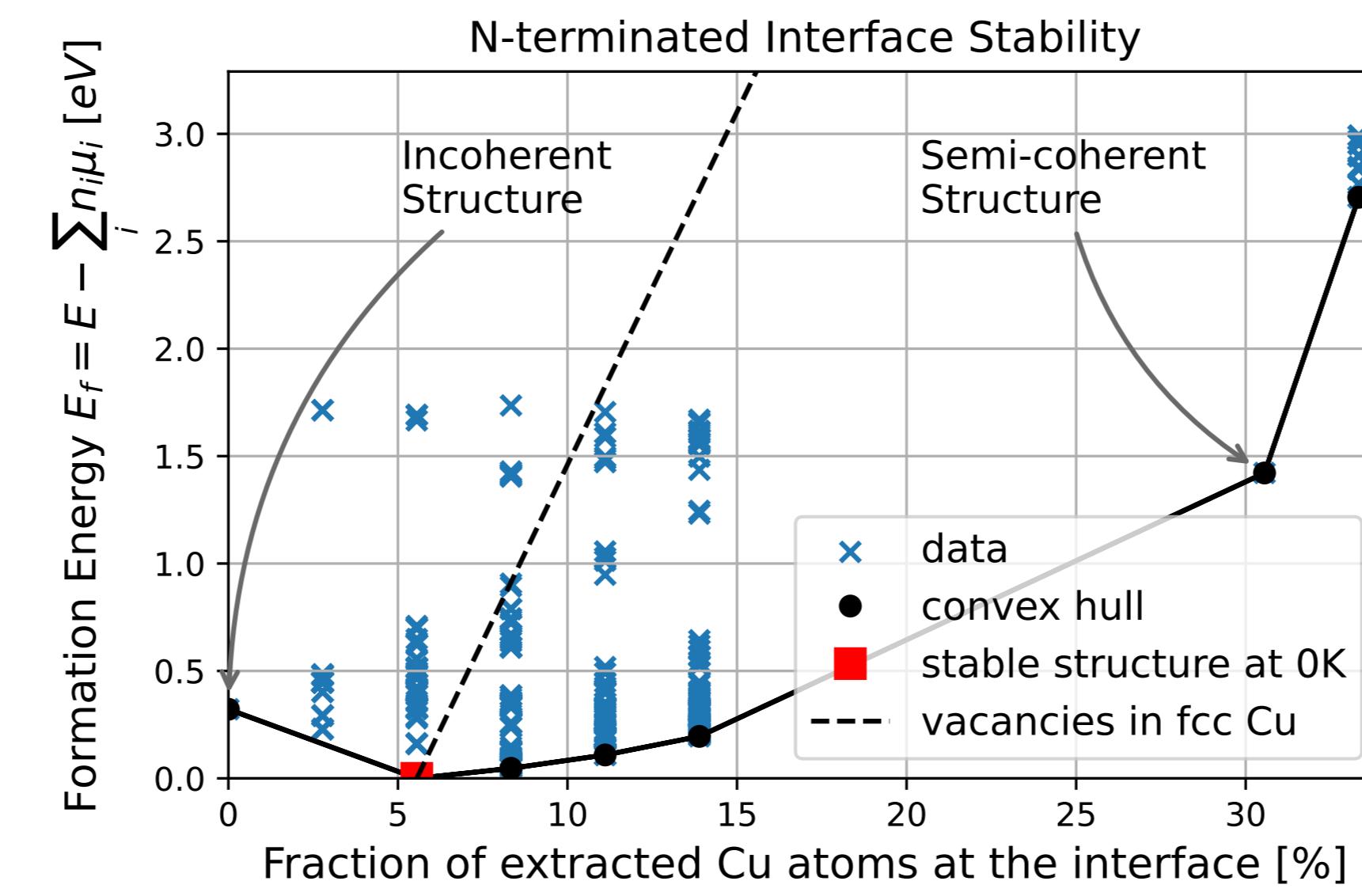


Figure 5: Formation energy as a function of the vacancy concentration at 0K.

- The stable N-terminated interface structure contains regions of bonded and unbonded Cu atoms.

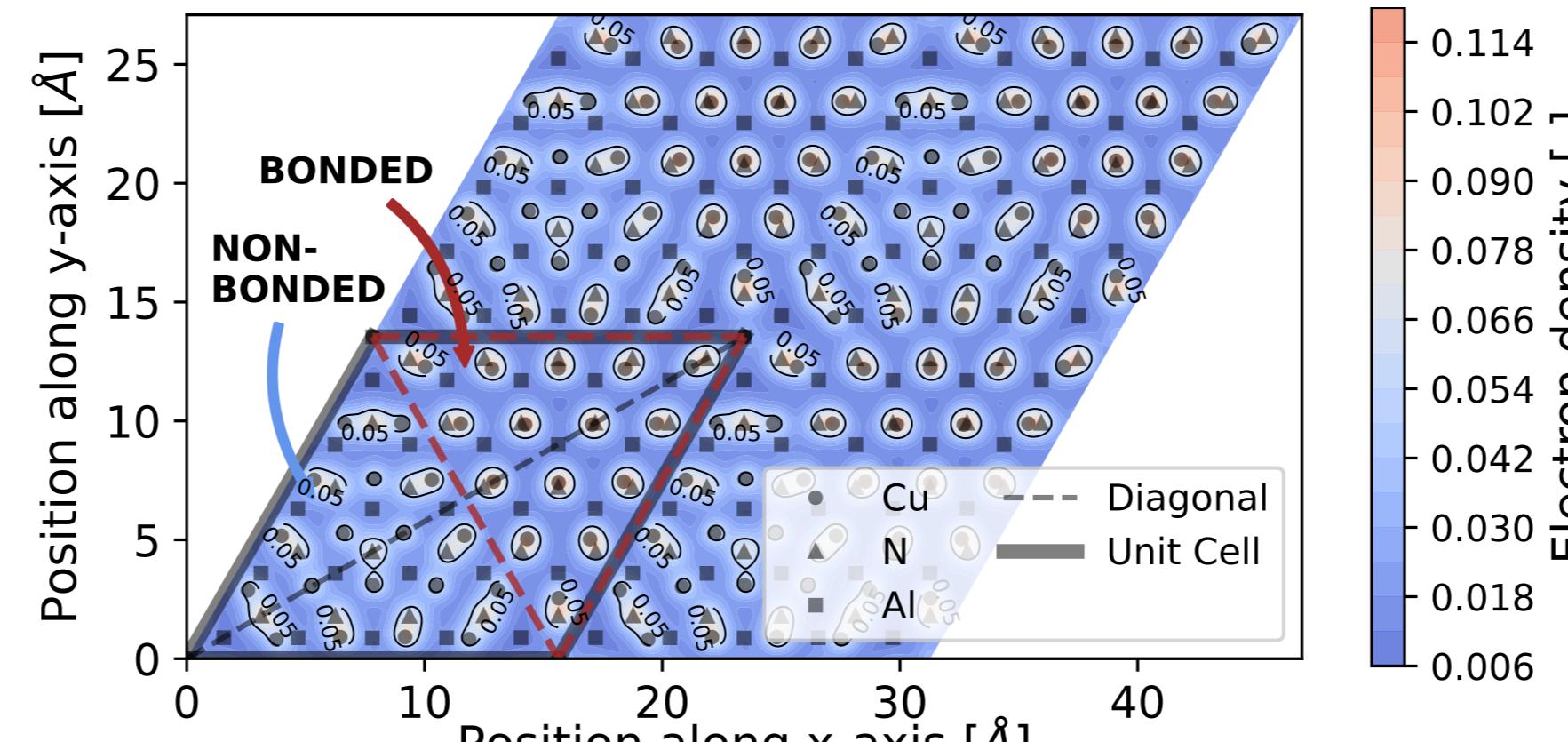


Figure 6: Electron density of the stable structure at the N-terminated interface.

Vacancy Migration

- Barrier-less vacancy migration from the bonded site to the nearest non-bonded sites suggests the presence of the trapping sites at the N-terminated interface.

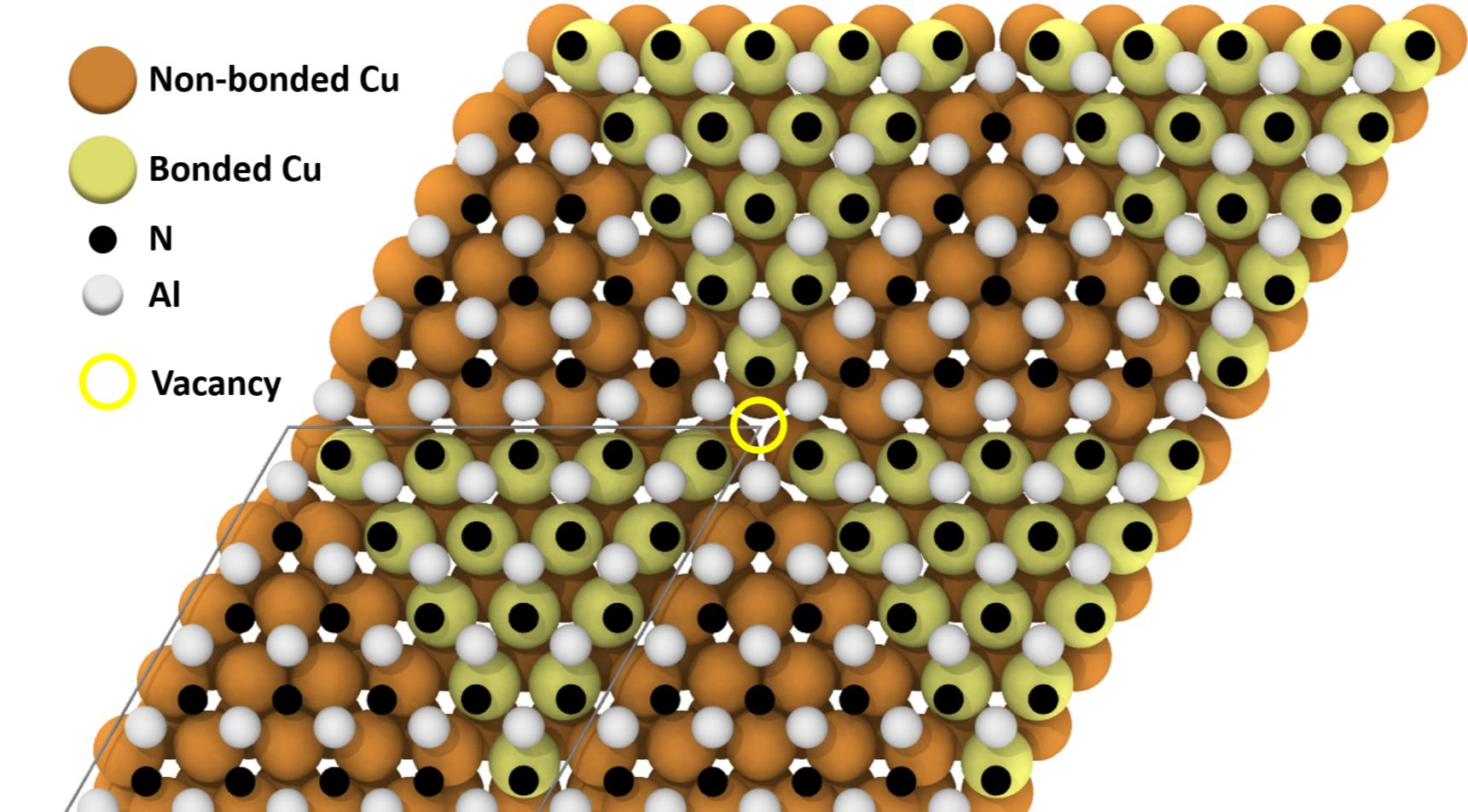


Figure 7: Possible vacancy-trapping non-bonded site at the N-terminated interface.

- In-plane vacancy migration is favored in the non-bonded regions of the N-terminated interface

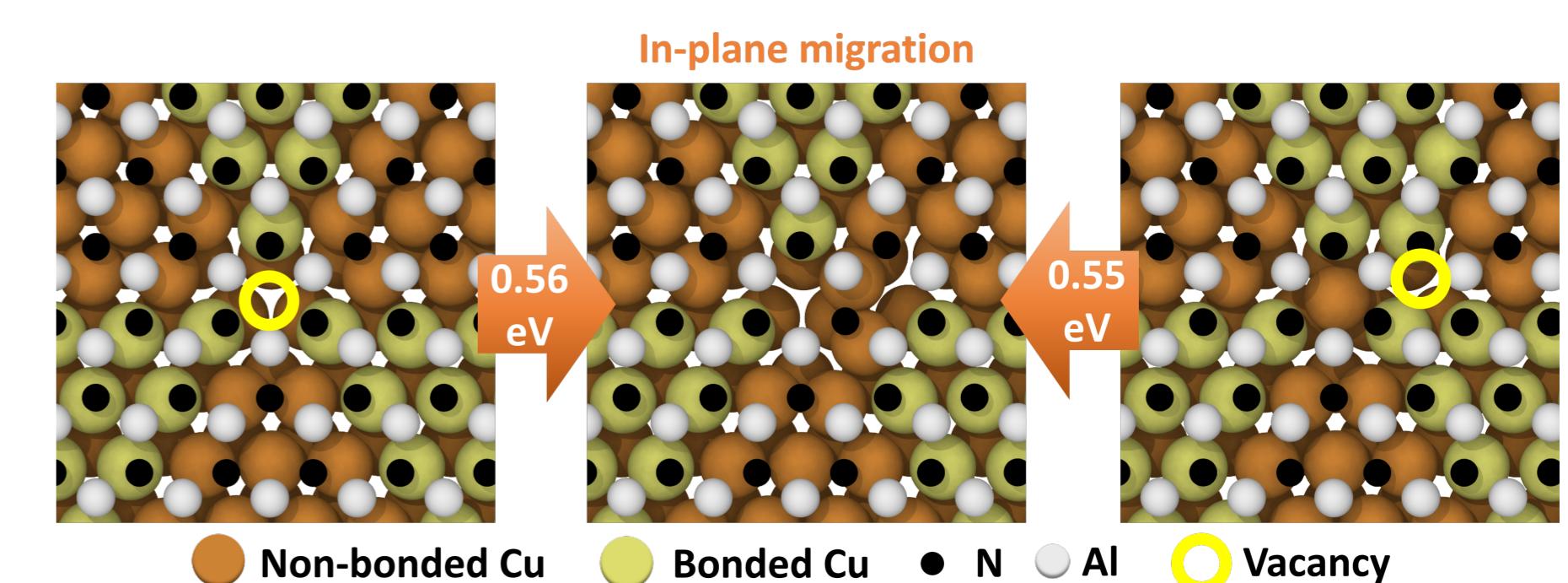


Figure 8: In-plane vacancy migration at the N-terminated interface represented by extreme case of the jump to the second neighbor shell.

- Out-of-plane vacancy migration energies suggest vacancy segregation to the non-bonded regions of the N-terminated interface

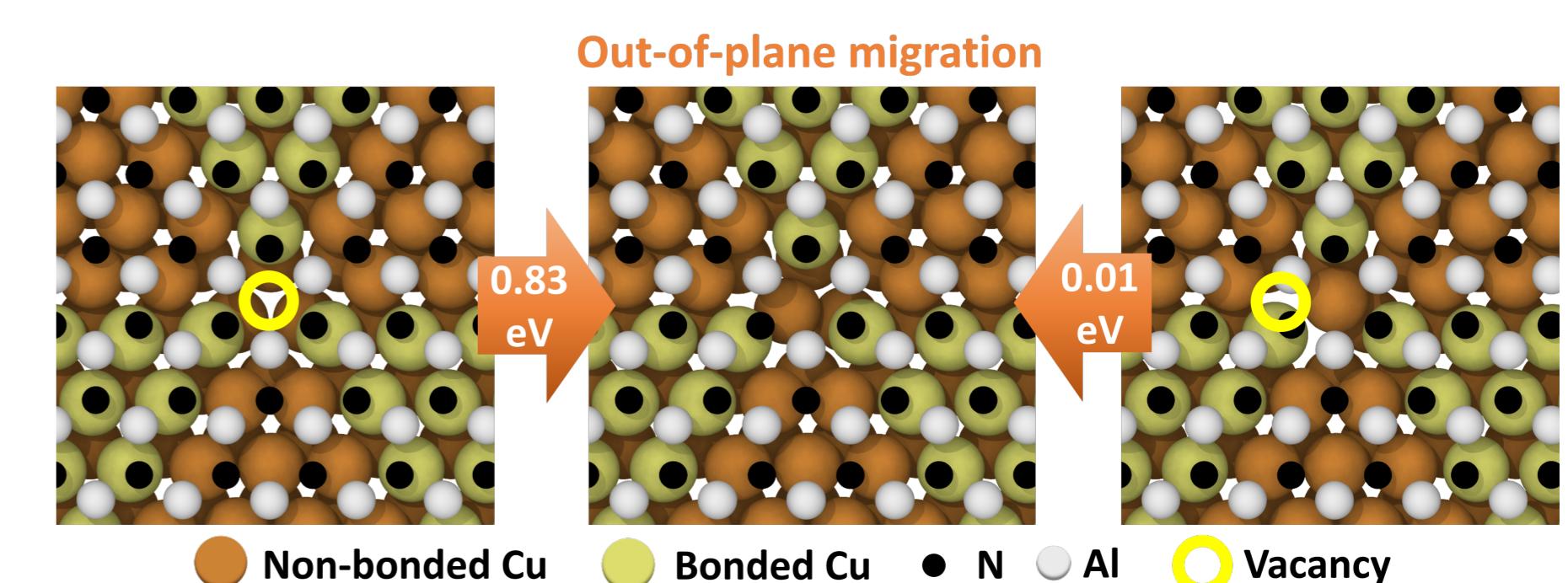


Figure 9: Out-of-plane vacancy migration at the N-terminated interface.

- Lower-than-bulk vacancy migration energies are observed near both N- and Al-terminated interfaces

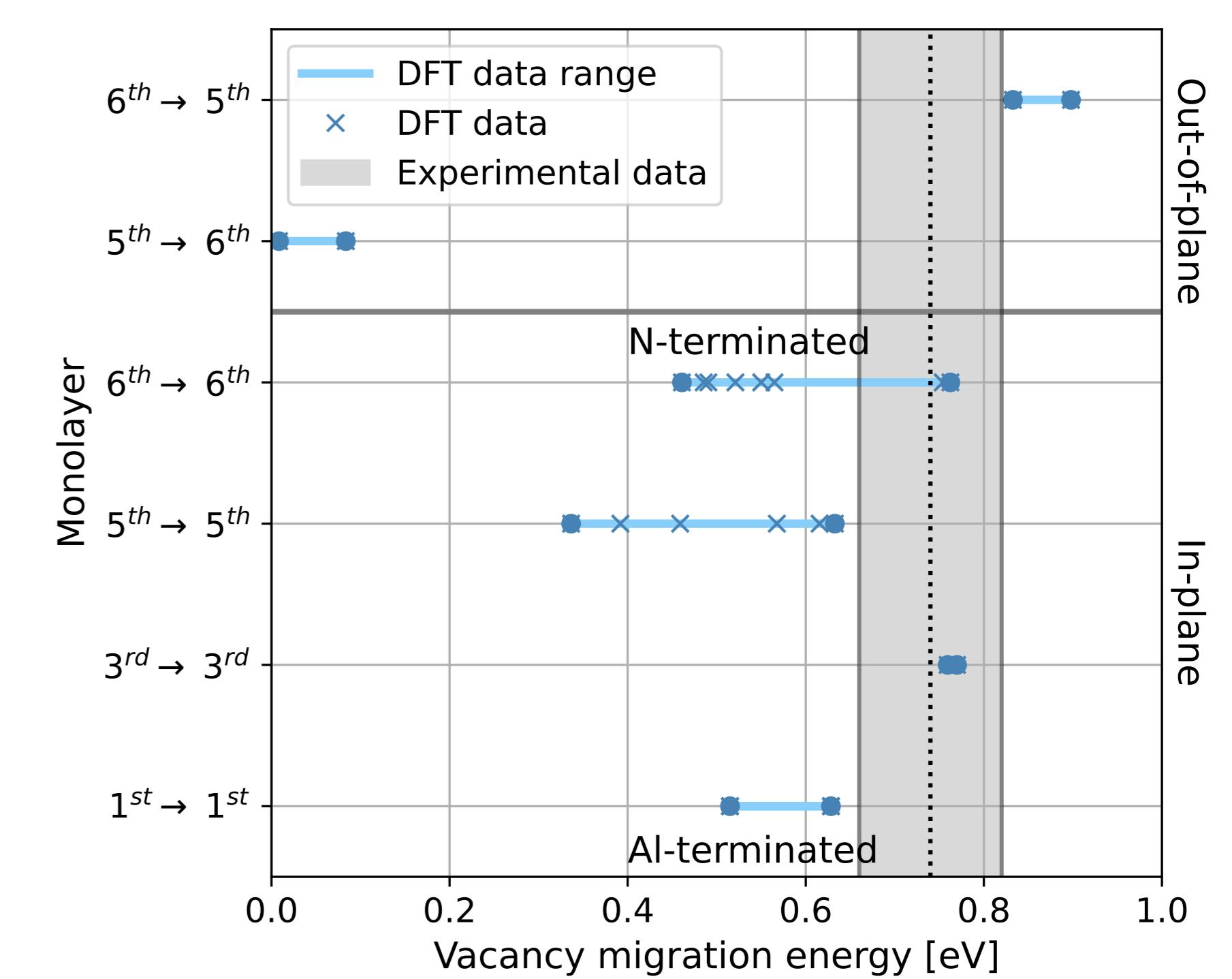


Figure 10: Sampled vacancy migration energies in the Cu slab. Grey region correspond to the bulk values from the literature [8].

Take-Home Message

Both Al- and N-terminated interfaces promote Cu diffusion by lowering vacancy formation and vacancy migration energies in neighboring Cu planes

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