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Motion dynamics of Si (100) positive and negative islands under electromigration and thermomigration

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Mass transport processes play an important role in nano devices. They determine the morphology and the stability of a working device, and eventually its lifetime. When a direct electric current is applied to a material, it affects the mass transport by adding a bias to the atomic diffusive motion. This effect, called electromigration, can play an important role on the dynamics and the morphological stability of nanostructures at surfaces. In this work we have studied the motion of single-step holes and islands under the effect of an electric field on Si(100), in real time, by Low Energy Electron Microscopy (LEEM). The details of the motion depend on the strong diffusion anisotropy of the Si dimer rows. Studying the velocity and the shape of the nanostructures, we discuss a model to explain and guide the motion of holes and islands.

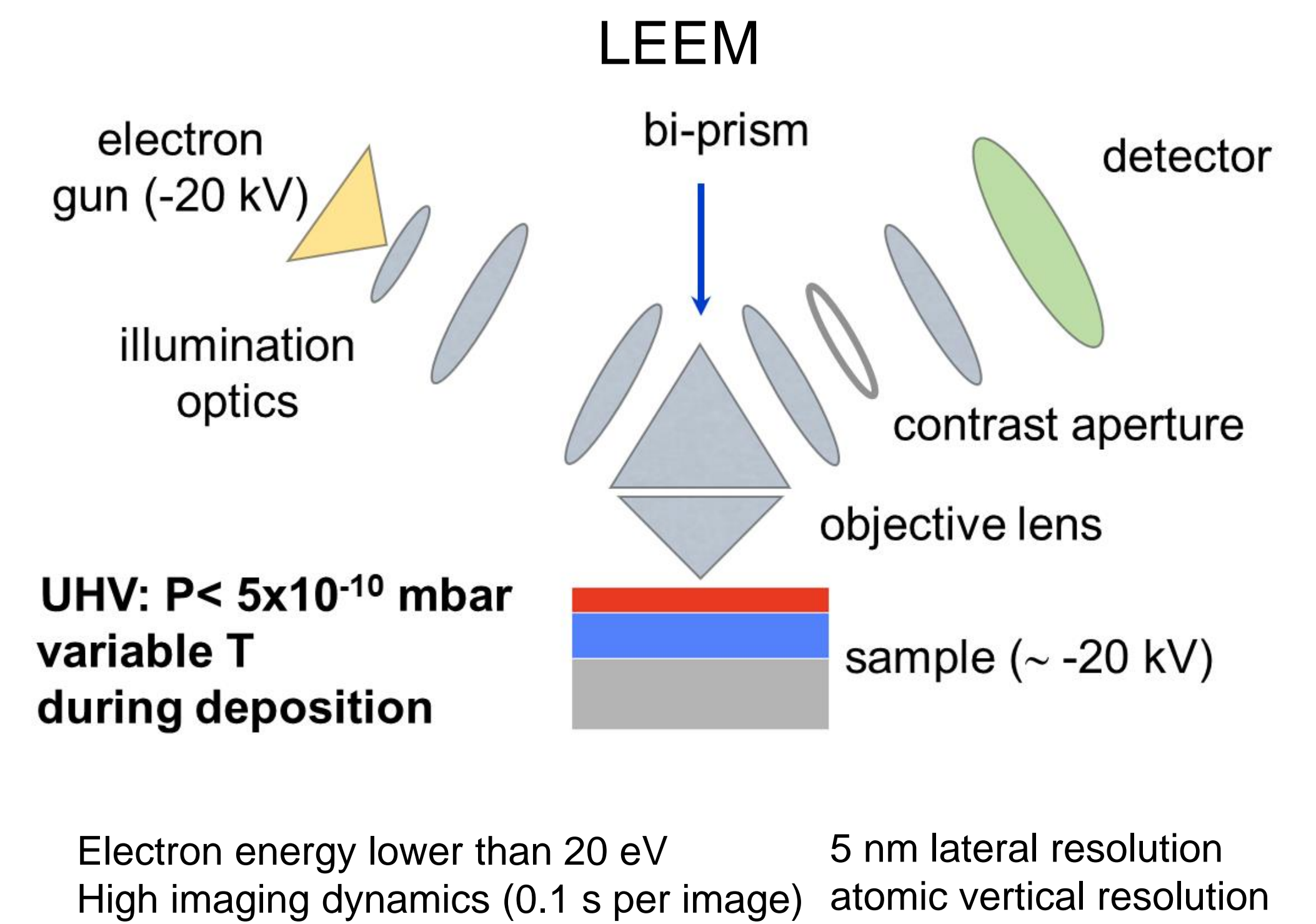
The manipulation of nanostructures is an important challenge for nanoelectronics and nanofabrication technologies. External fields and thermal gradients are natural candidates to move and control the nanostructure position on a surface. Particularly promising is the use of electric fields to induce mass transport in specific directions, phenomenon known as electromigration (EM).

The elementary process of **electromigration** of an atom on a surface (adatom) is well known: the **electric current biases random diffusion** inducing mass transport in specific directions. The motion of many adatoms results in the motion of an entire nanostructure.

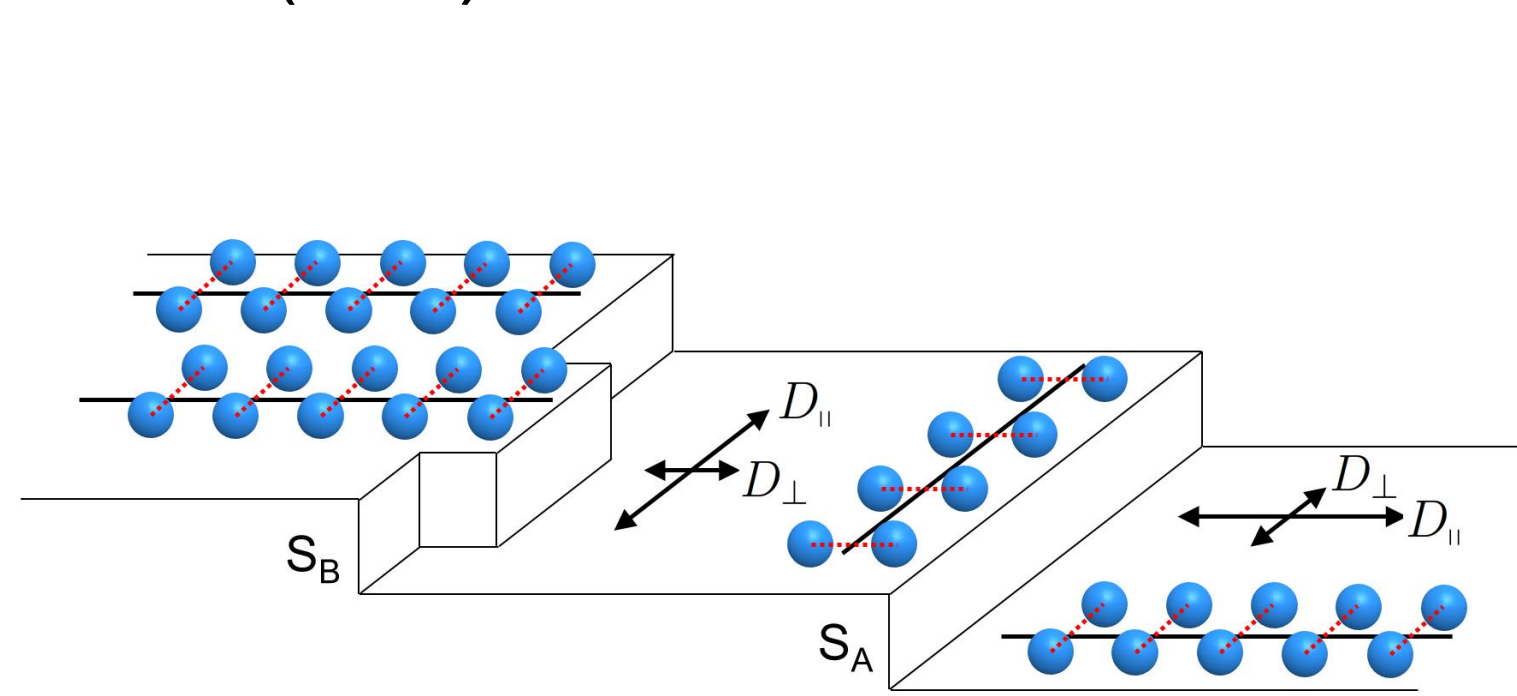
While it has been neglected in most studies, the **crystalline anisotropy** of the surface may play an important role on adatom motion and therefore on nanostructure motion.

We have used Low Energy Electron Microscopy (**LEEM**), to observe Si(100) surfaces in-situ and in real time with high temporal and spatial resolution, and in a large temperature range (1000-1500 K).

In order to support the experimental results and obtain more insights in the motion mechanism, we have developed a **Kinetic Monte Carlo model** based on both anisotropic and electromigration-biased diffusion at surfaces.

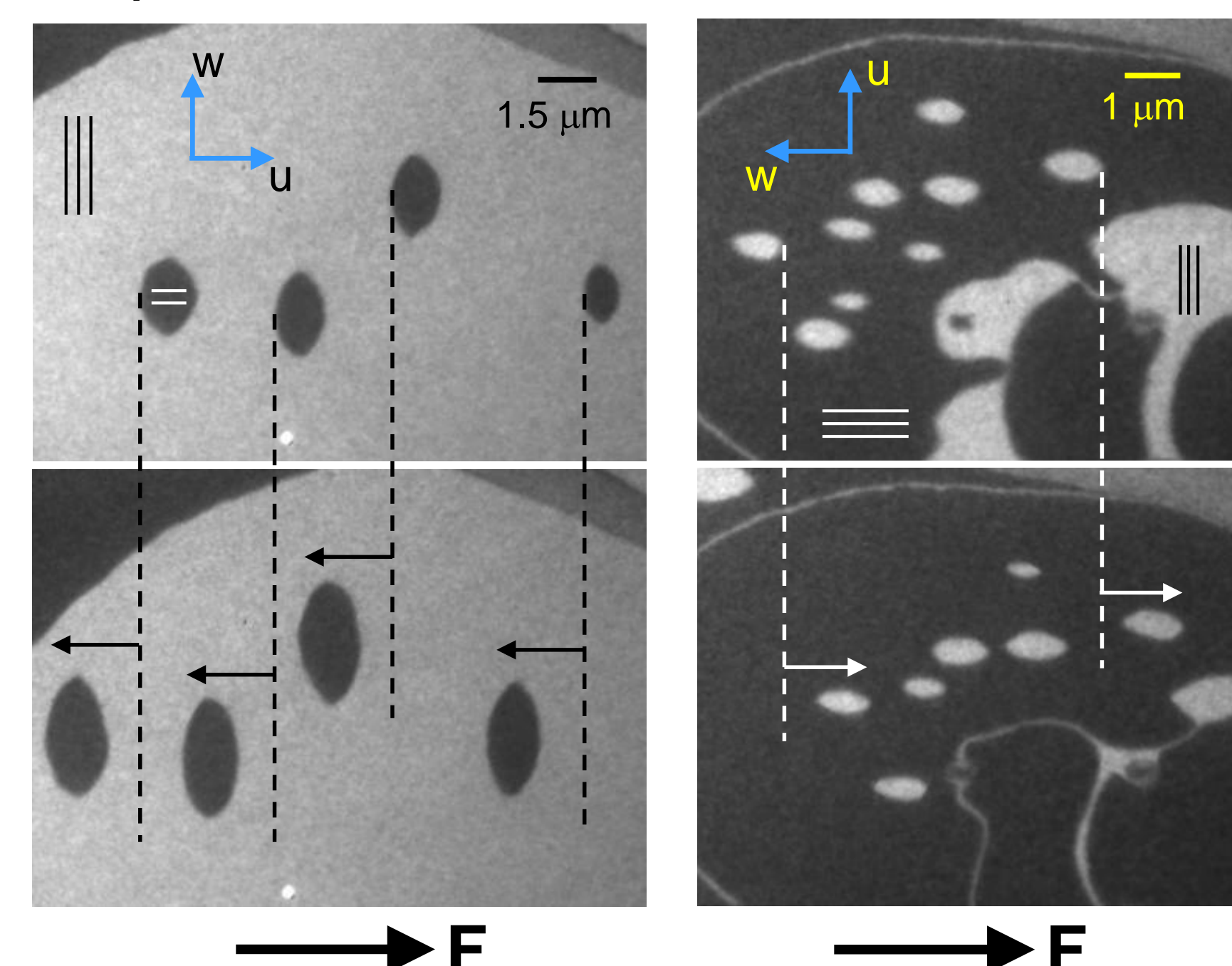


Si(100) surface reconstruction



The Si(100) surface structure has dimer rows running perpendicularly on alternating terraces. **Diffusion is faster along dimer rows** than perpendicularly to them

Displacement of 2D voids under electromigration (EM)

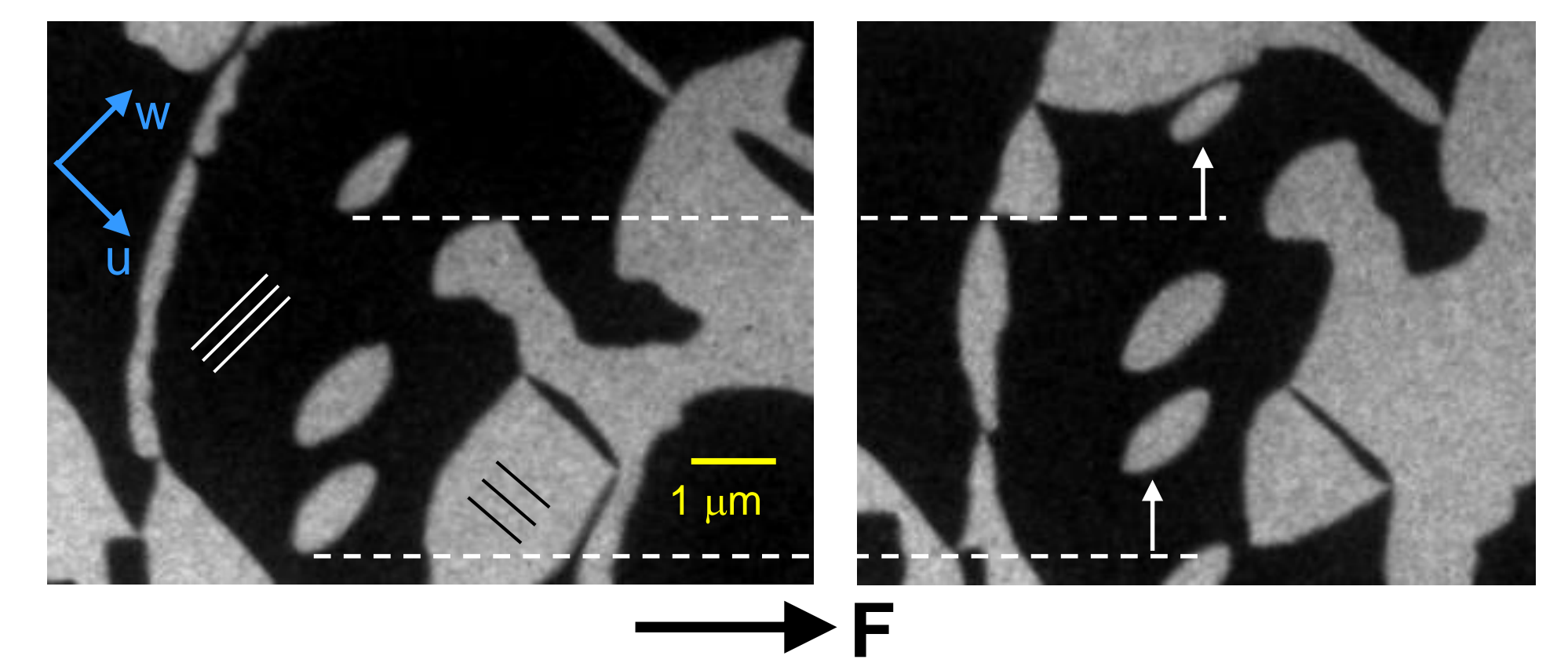


The **shape** of the voids depends on the **orientation of the dimer rows** of the upper terrace (outside the voids)

Void elongated **perpendicularly** to the EM force move **opposite** to the force

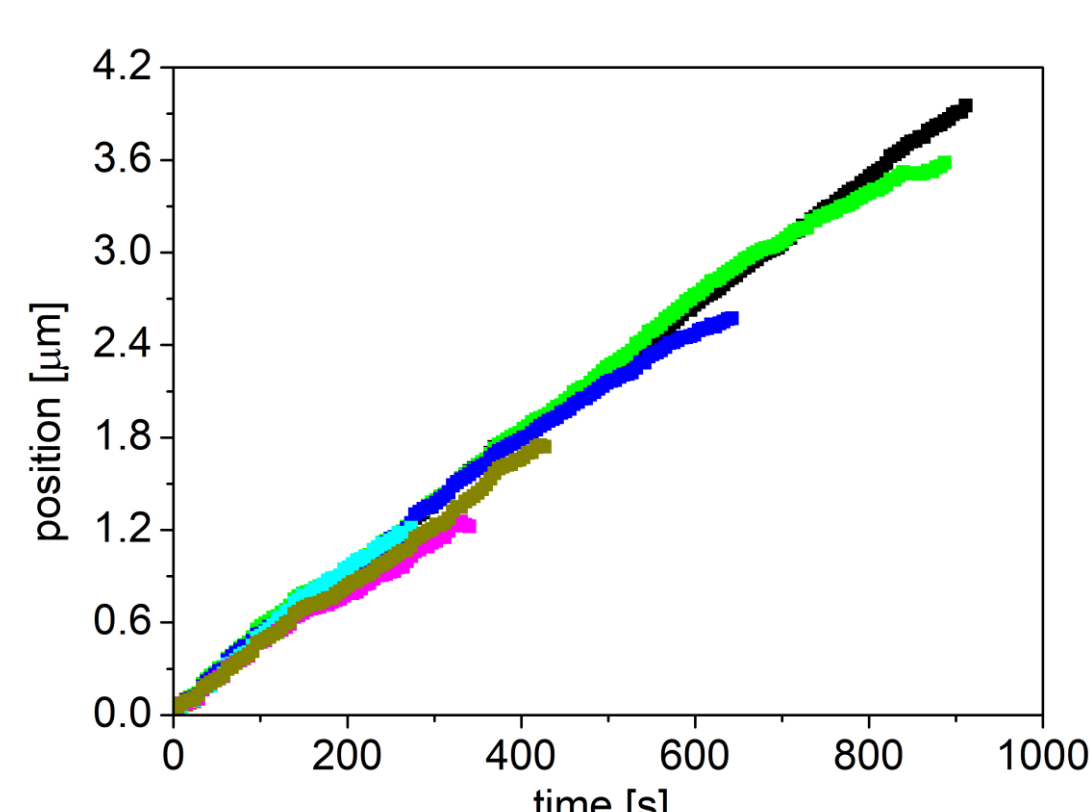
Void with shape **parallel** to the force move **in the same direction** of the force

Current at 45° from the dimer rows



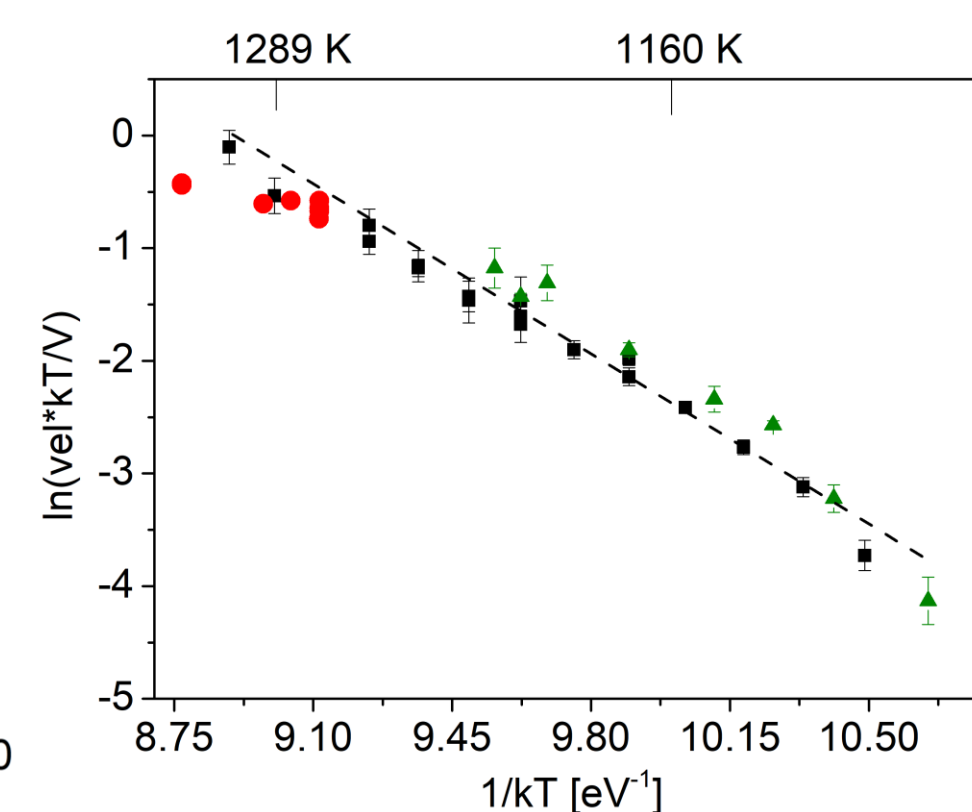
With a force applied from left to right, the voids move towards the top, at 90° from the electric-field direction and 135° from the [011] axis

Void velocity (EM)



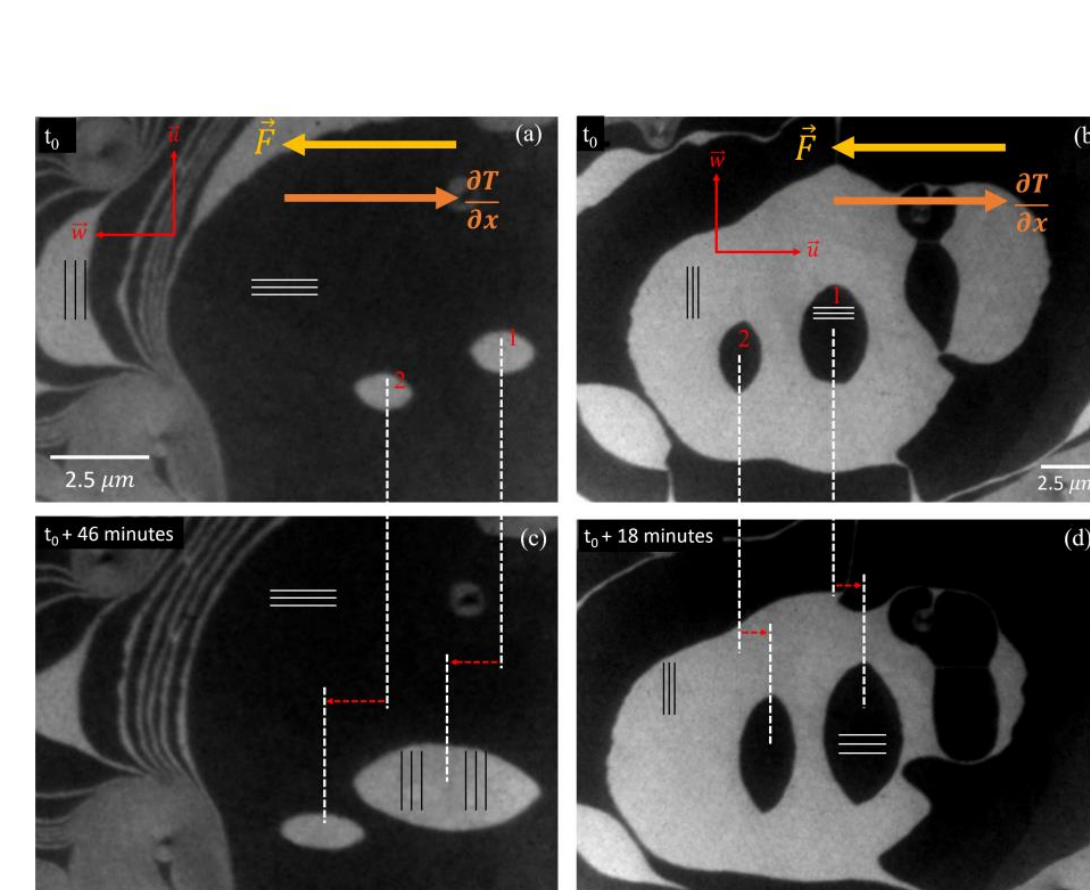
Position as a function of time of seven voids at 1150 K, they have the **same velocity**

Activation energy



The effective activation energy for the void motion is **2.0 ± 0.1 eV**

Displacement of voids under thermomigration

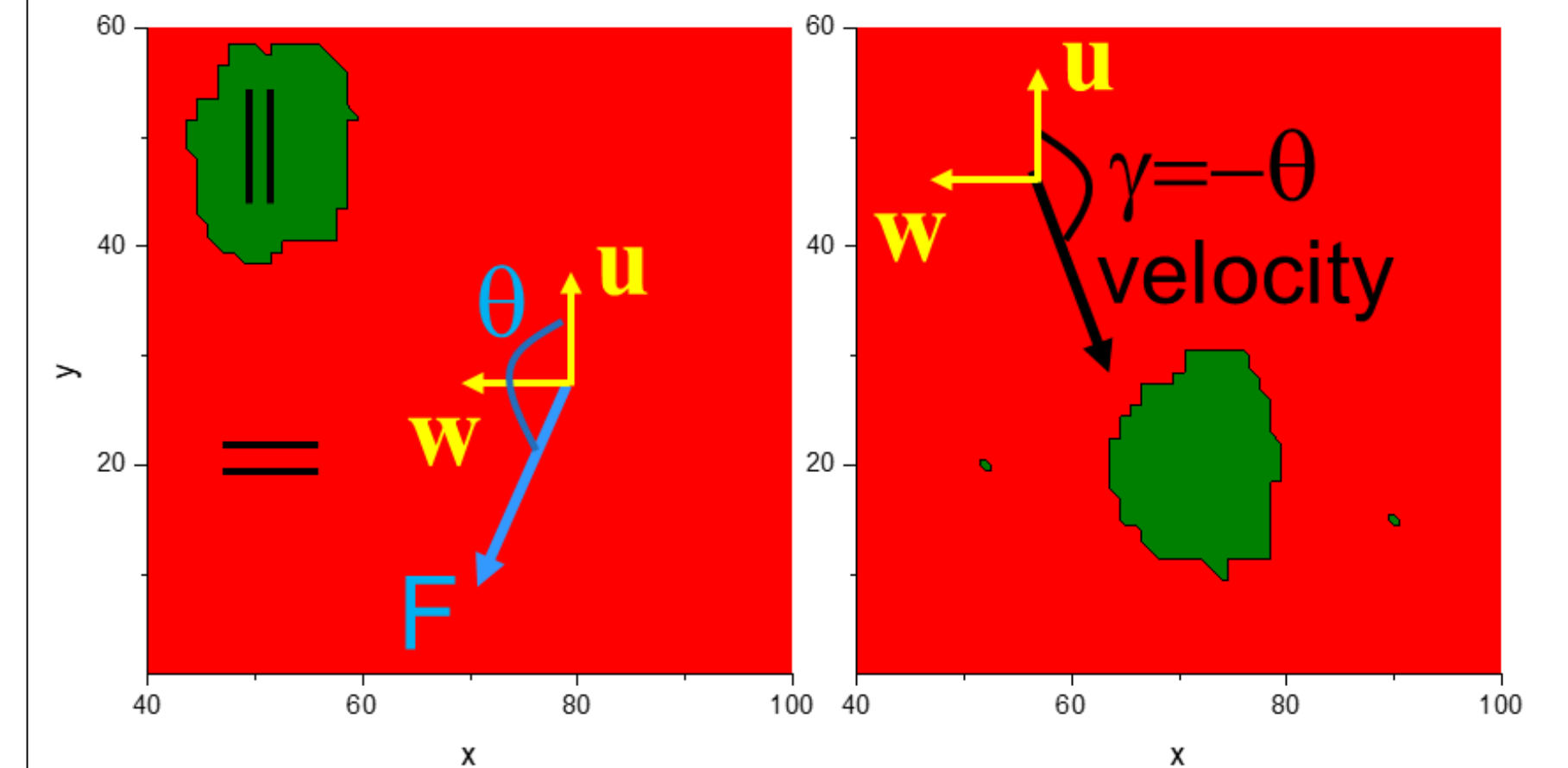


2D voids moving under thermomigration (TM), the **left side is colder than the right side**

Ad-dimers (presumed mobile species) move from the hot to the cold side

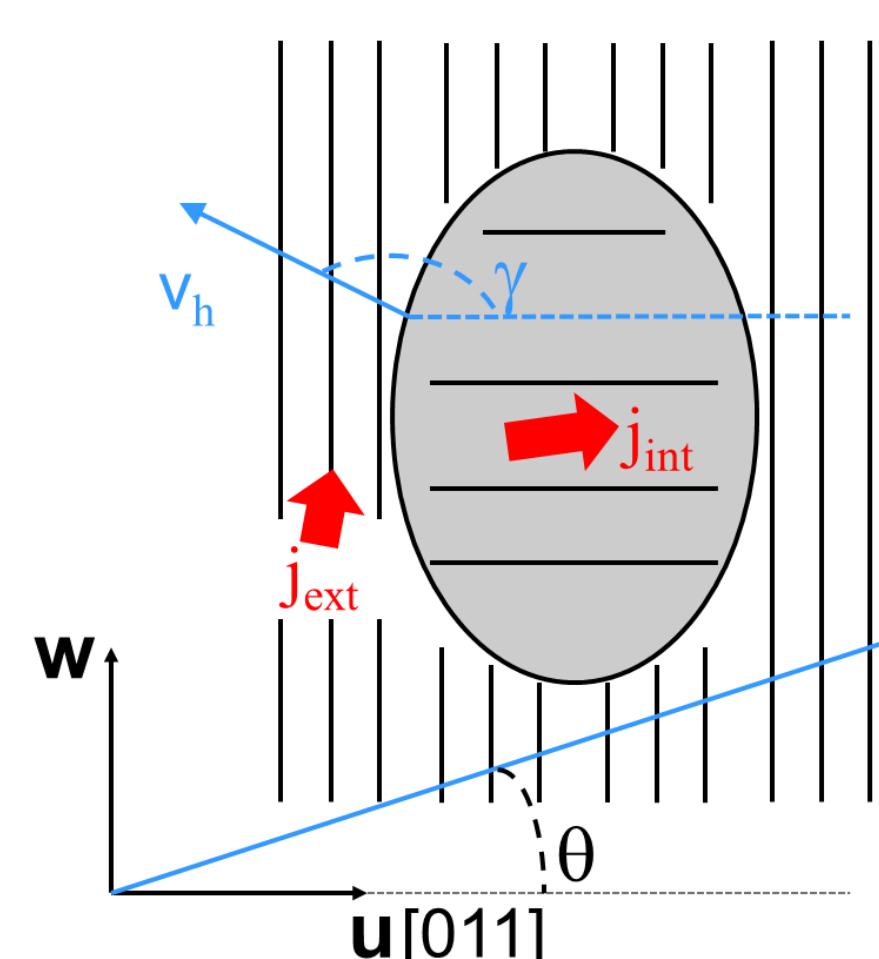
Motion of voids and islands similar to EM

KMC simulations



Kinetic Monte Carlo simulations taking into account the dimer rows and the diffusion anisotropy **reproduce all the observed behaviors** of void and island motion

Void motion model



$$\vec{F} = Z^* \cdot e \cdot |E| \cdot (\cos\theta \vec{u} + \sin\theta \vec{w})$$

$$\vec{v}_h = a^2 \cdot (\vec{j}_{ext} - \vec{j}_{int})$$

$$\vec{j}_{ext} = A \cdot (D_{\perp} \cdot \cos\theta \cdot \vec{u} + D_{\parallel} \cdot \sin\theta \cdot \vec{w})$$

$$\vec{j}_{int} = A \cdot (D_{\parallel} \cdot \cos\theta \cdot \vec{u} + D_{\perp} \cdot \sin\theta \cdot \vec{w})$$

$$\vec{v}_h = A \cdot a^2 (D_{\parallel} - D_{\perp}) \cdot (-\cos\theta \cdot \vec{u} + \sin\theta \cdot \vec{w})$$

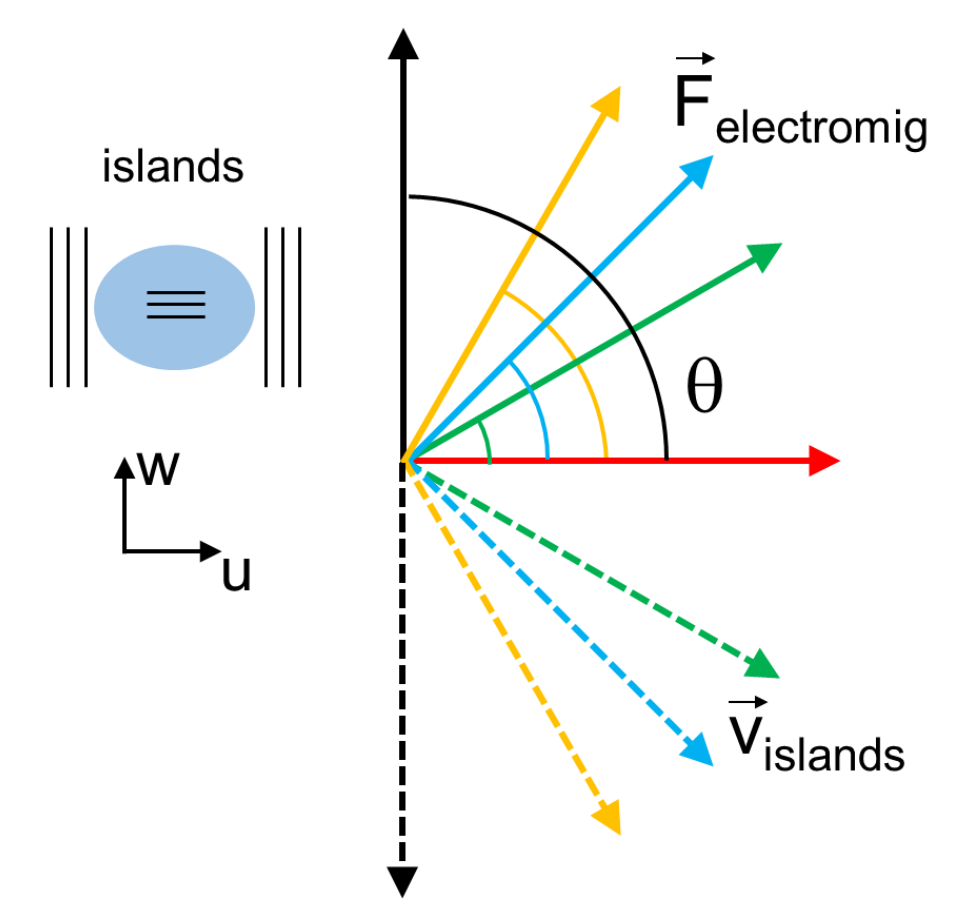
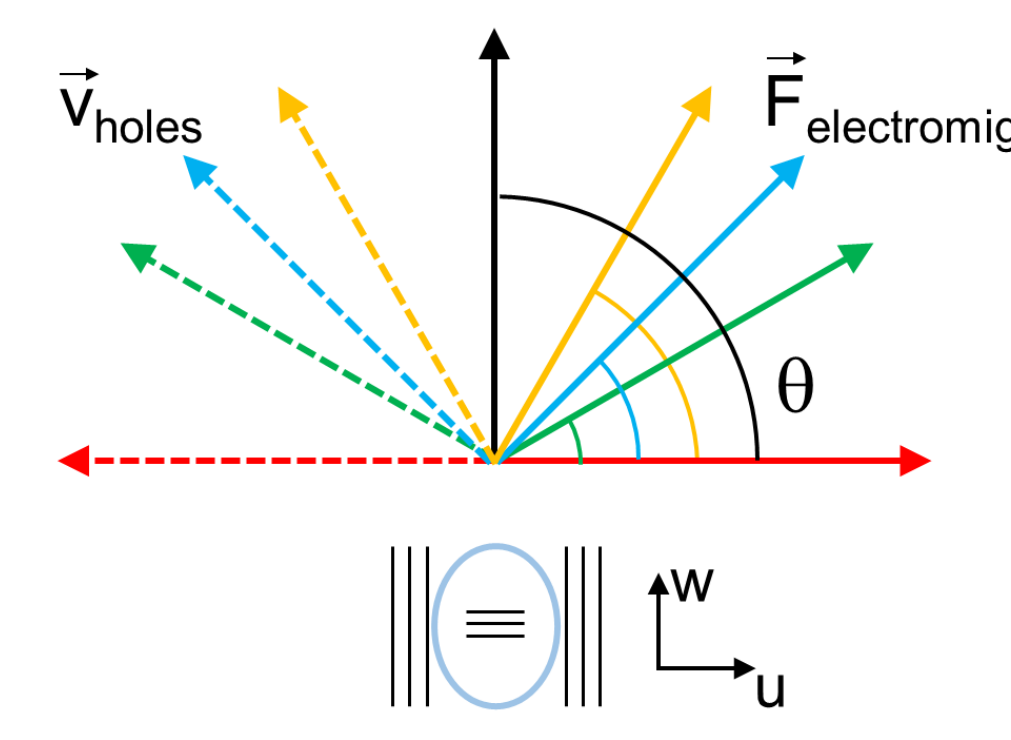
$$\vec{v}_{isl} = A \cdot a^2 (D_{\parallel} - D_{\perp}) \cdot (\cos\theta \cdot \vec{u} - \sin\theta \cdot \vec{w})$$

$$A = c \cdot \frac{Z^* \cdot e \cdot |E|}{kT}$$

$$\vec{v} = |v| \cdot (\cos\gamma \cdot \vec{u} + \sin\gamma \cdot \vec{w})$$

$$\text{for voids: } \gamma = 180^\circ - \theta$$

$$\text{for islands: } \gamma = -\theta$$



Schematics of a 2D void.

The dimer rows inside the hole are oriented horizontally, in the same direction of **u**. The force exerted by the electric field is oriented along the blue arrow and forms an angle **theta** with **u**.

The void displaces in a direction forming an angle gamma with u.

J_ext and **J_int** are the atomic fluxes at the exterior and at the interior of the void. **D** are diffusion coefficients parallel and perpendicular to dimer rows; **v** are hole and island velocities; **a** is an atomic length; **c** is the concentration of diffusion species

Motion direction of holes and islands for different force directions

Conclusions

- The motion of nanostructures on Si(100) is possible thanks to the difference of diffusion coefficient parallel or perpendicular to dimer rows.
- The effective activation energy for the motion of 2D islands and voids at Si(100) surfaces is 2.0 ± 0.1 eV, given by the sum of a diffusion energy and a creation energy of the diffusing species