# Ab-initio and STM investigation of the $Nd_2Fe_{14}B$ surface

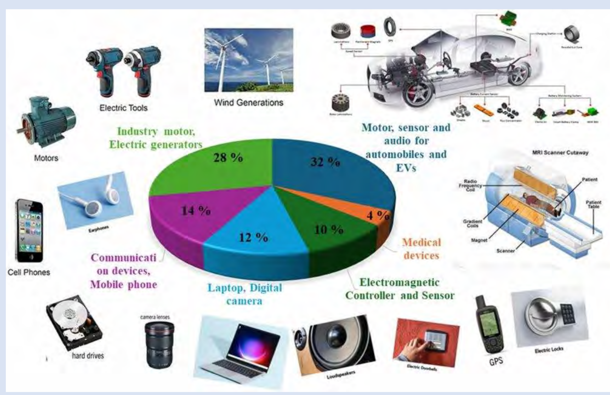
**Sana Saeed[1], Willfried Bajoun Mbajoun[2], Abhirami Suresh[2], Vincent Fournée[2], Julin Ledieu[2], Matej Komelj[1], Kristina Žužek[1], Sašo Štrum[1],**

1: Jožef Stefan Institute, Department for Nanostructured Materials, Jamova cesta 39, SI-1000 Ljubljana, Slovenia

2: Institute Jean Lamour, Campus Artem, 2 allée André Guinier, 54011 Nancy, France

## Inroduction:

- $Nd_2Fe_{14}B$ (Neodymium-Iron-Boron) based permanent magnets are essential in various technologies.
- $Nd_2Fe_{14}B$ in theory exhibits exceptionally high magnetocrystalline anisotropy, real magnets often fail to reach this intrinsic potential.
- The coercivities observed in Nd-Fe-B permanent magnets represent only 20% of what is theoretically possible, which means that significant improvements are possible. $Nd_2Fe_{14}B$ surfaces are often regarded as the source of a degraded magnetic performance.
- In this work, we examine the surface structure of $Nd_2Fe_{14}B$ single crystals and present a combined experimental and computational characterization of the $Nd_2Fe_{14}B$(001) surface..



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## Objectives:

### 1 Surface Atomic Structure

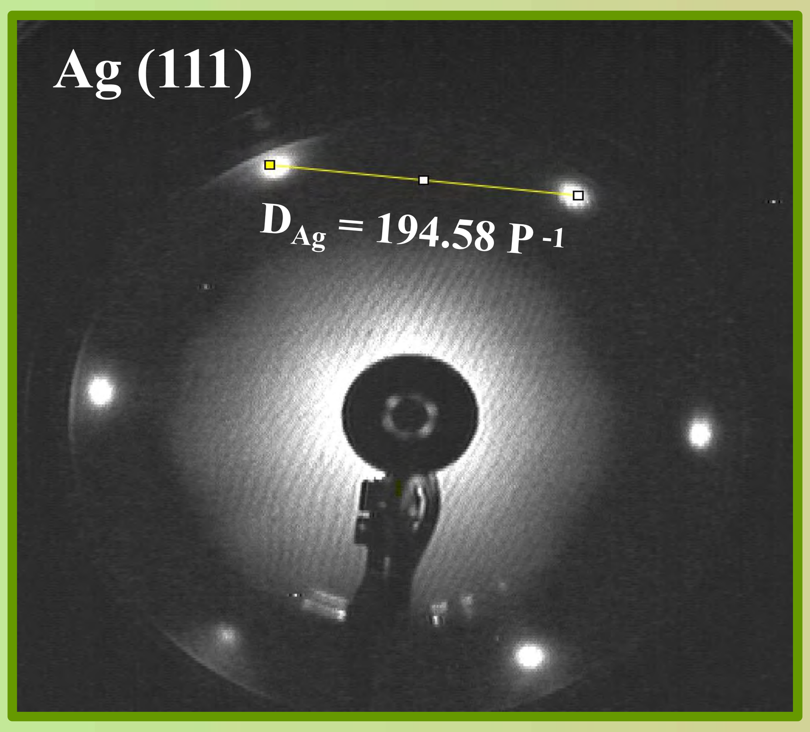
▶ Characterize the surface of single-crystal $Nd_2Fe_{14}B$ using STM and LEED.

▶ Interpret contrast variations in STM images as changes in local density of states (LDOS).

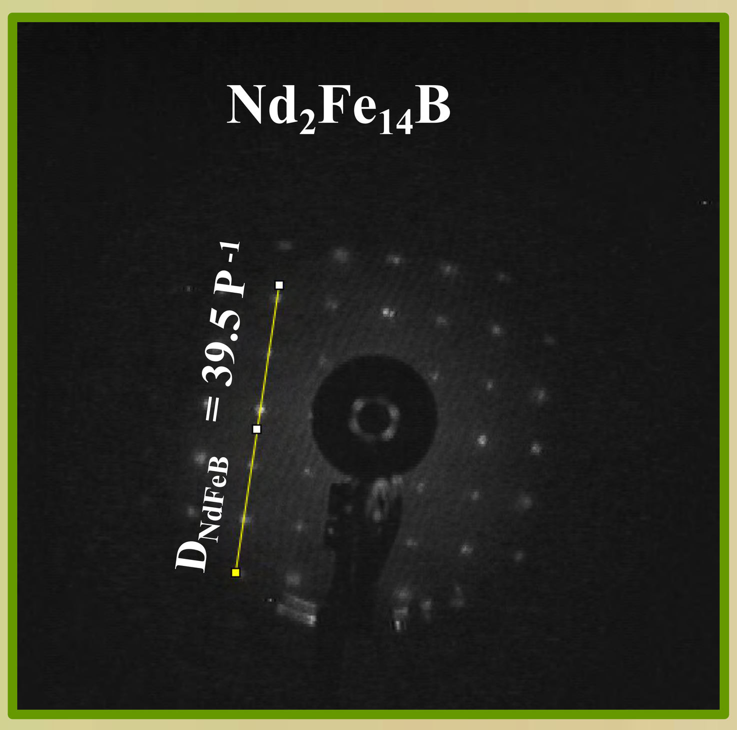
### 2 DFT-Based Theoretical Modeling

▶ Set the stage for Density Functional Theory (DFT) to model:

- Surface energetics
- Calculate the simulated STM images





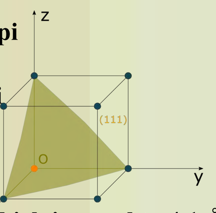




$||a_1||\,.\,||a_1^*||$ x cos 30°= 2pi

$||a_1||\,.\,||a_1^*||$ x $\sqrt{3}/2$= 2pi

$||a_1^*||$ = 4pi/ {$\sqrt{3}$ ($a_{Ag}\sqrt{2}/2$ )}



$a_{Ag}$ is bulk lattice parameter of Ag which is equal to 4.1 Å

$||a_1^*||$ = 2.5 A-1

$D_{Ag}$ → 194.58 P -1

$D_{NdFeB}$ → 39.5 P -1

$$a_{Nd2Fe14B} = a_{Ag,known} \times \frac{D_{Nd2Fe14B}}{D_{Ag}}$$

$a_{NdFeB*}$ = 2.5 A-1 (39.5 P -1 )/ 194.58 P -1

$a_{NdFeB*}$ = 0.50 A-1

this is in reciprocal space so for real space

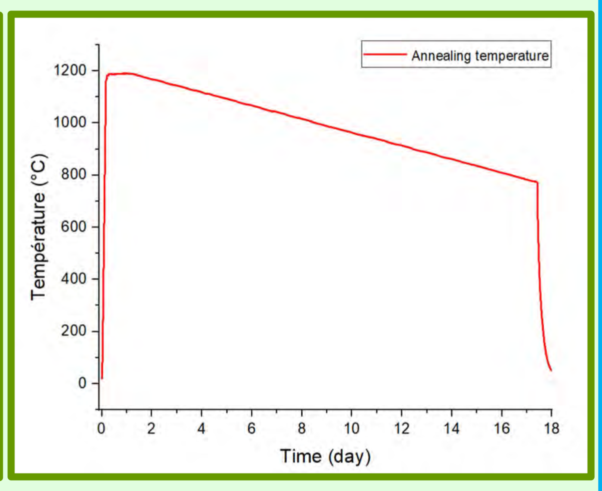
$a_{NdFeB}$ = 2pi/ a*

$a_{NdFeB}$ = 12. 5 Å

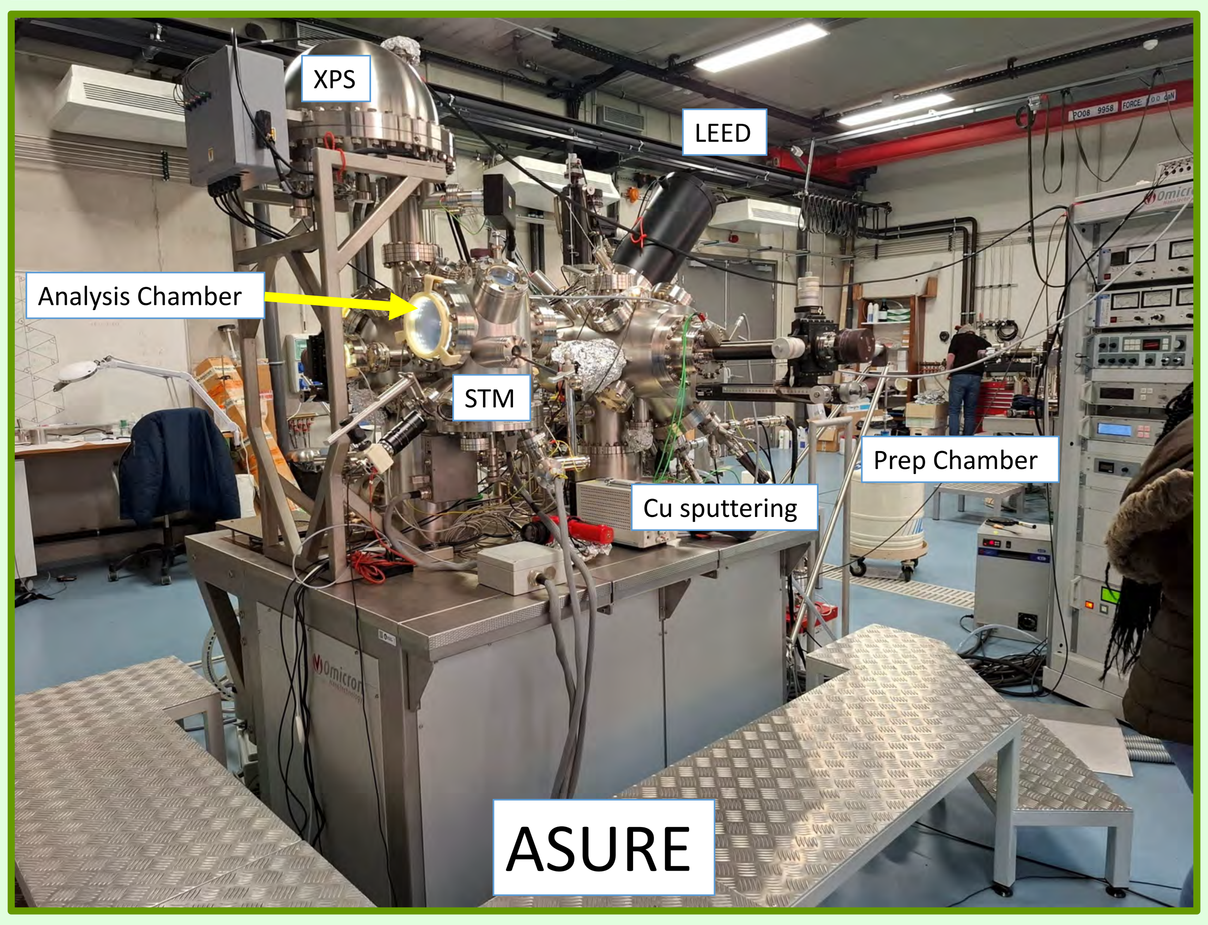
## Material and Synthesis:

### $Nd_2Fe_{14}B$ Self-flux method

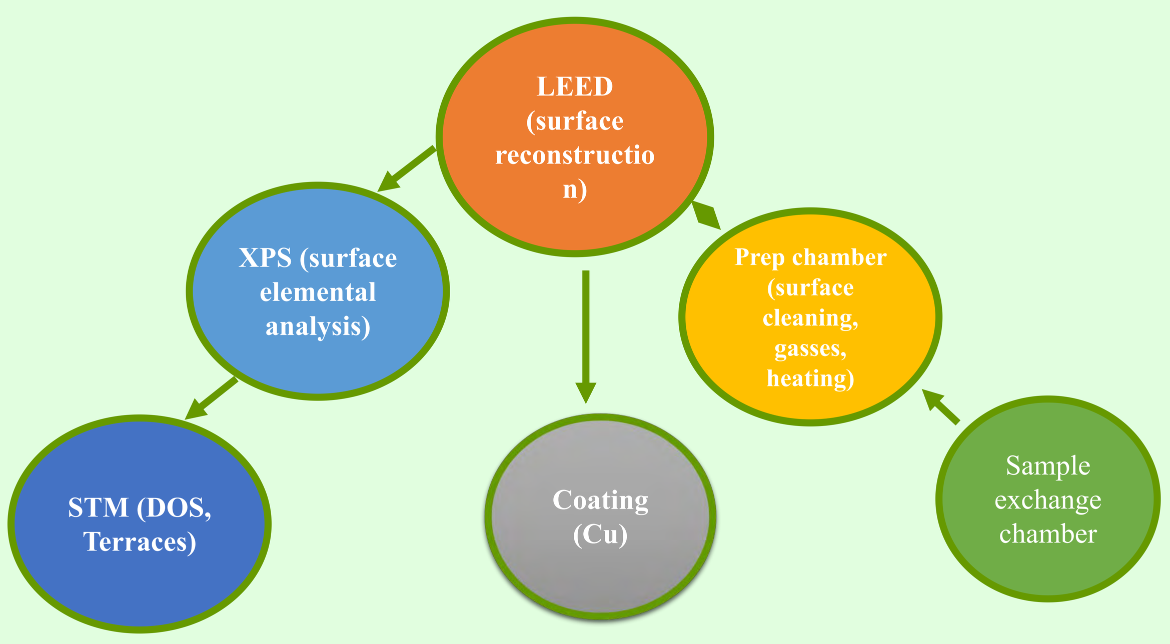
| Parameter | Total | Nd | Fe | B |
|---|---|---|---|---|
| Atomic % | 100.000 | 40.000 | 56.000 | 4.000 |
| Molar Mass (g/mol) | | 144.242 | 55.845 | 10.811 |
| Melting Temperature (°C) | | 1016 | 1538 | 2075 |
| Atomic % * Molar Mass | 8940.244 | 5769.680 | 3127.320 | 43.244 |
| Mass % | 1.000 | 0.64536 | 0.34980 | 0.005 |
| Desired Mass (g) | 4.200 | 2.711 | 1.469 | 0.020 |
| Weighed Mass (g) | 4.199 | 2.710 | 1.469 | 0.020 |



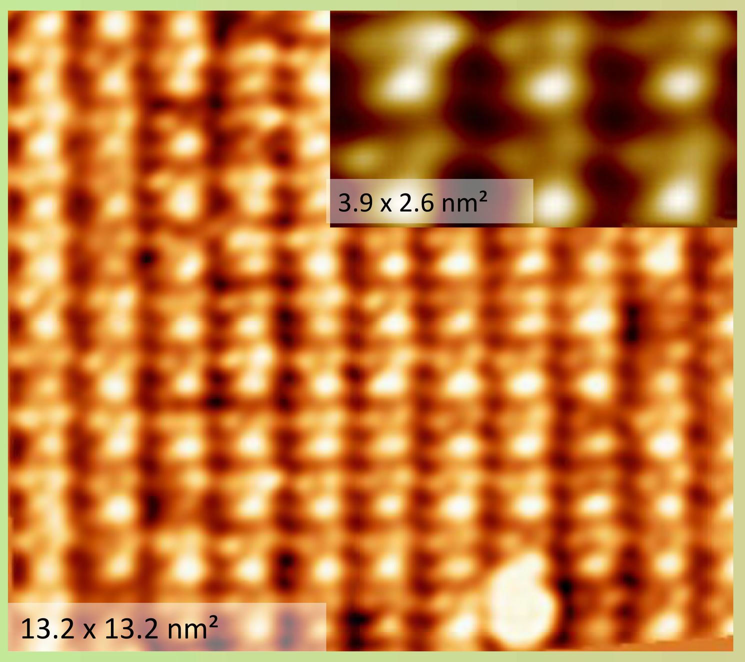






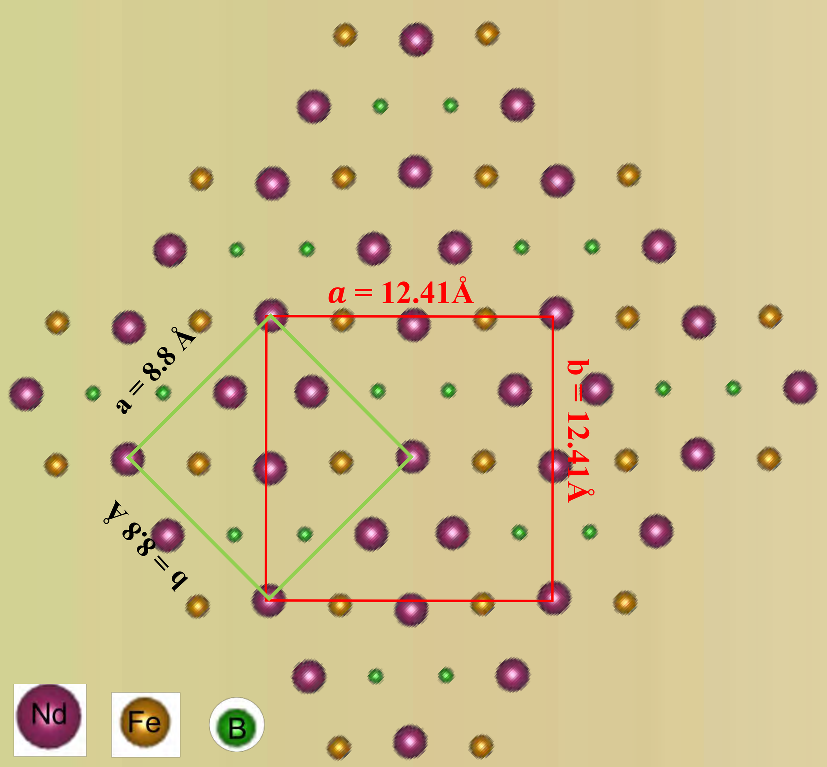








STM image of $Nd_2Fe_{14}B$ single crystal





Atomic arrangement of the $Nd_2Fe_{14}B$ (001) surface.

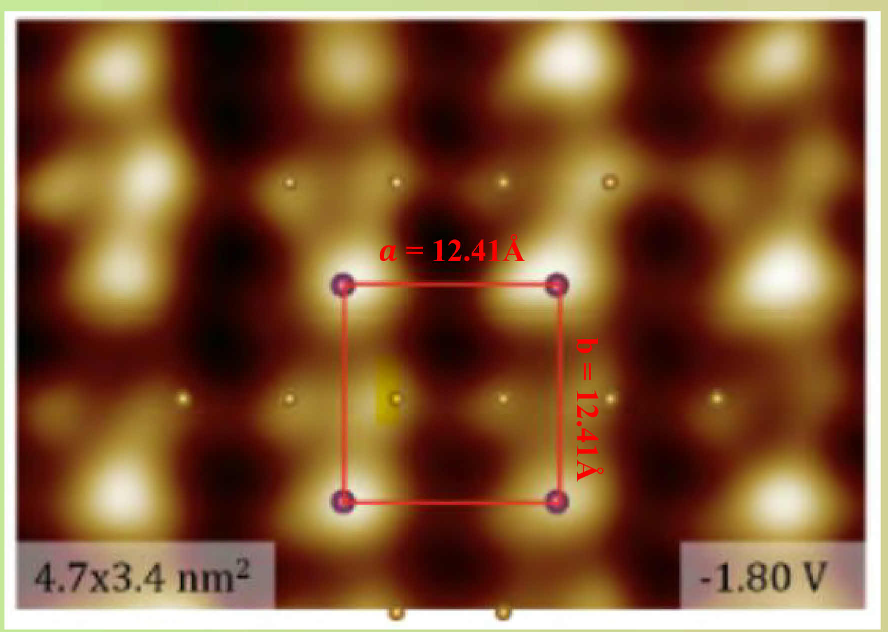
By Fast four Transform (FFT) analysis surface lattice parameter is measured to be a=b=12.41 Å, indicating C($\sqrt{2} \times \sqrt{2}$, 45°) surface reconstruction. The same result is confirmed by LEED.

The mechanism yielding the surface reconstruction:

- Minimization of the surface free energy
- Relaxation of Surface Atoms
- Adsorbates and Defects

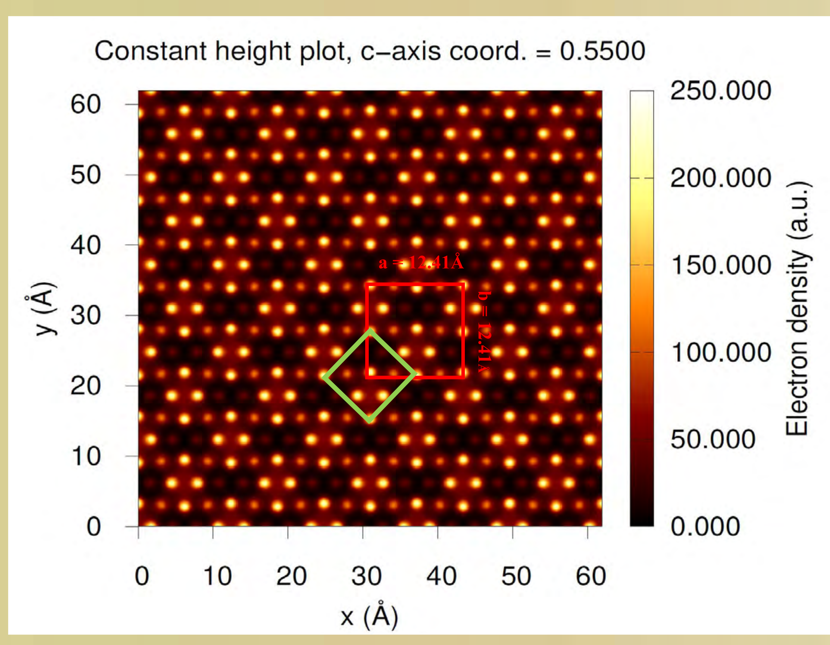
STM results demonstrate that the $Nd_2Fe_{14}B$ surface is atomically ordered and undergoes a well-defined surface reconstruction, which is an important step toward understanding its surface and properties.

**Atomic arrangement of the $Nd_2Fe_{14}B$ (001) surface. The green square represents the original 1×1 surface unit cell, while the red square shows the larger c(2×2)R45° surface reconstruction**





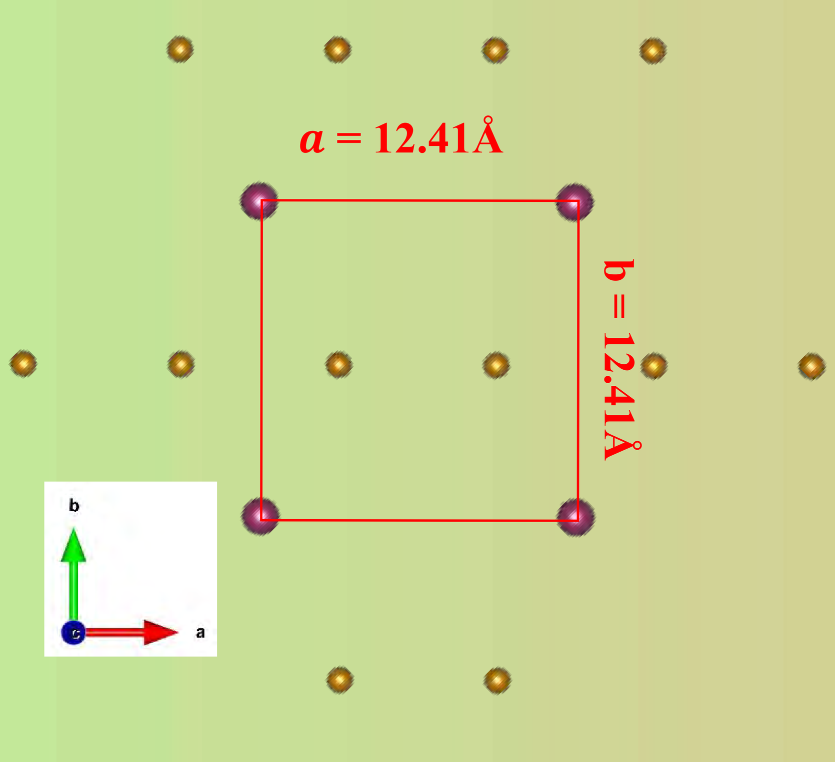
Experimental STM Image





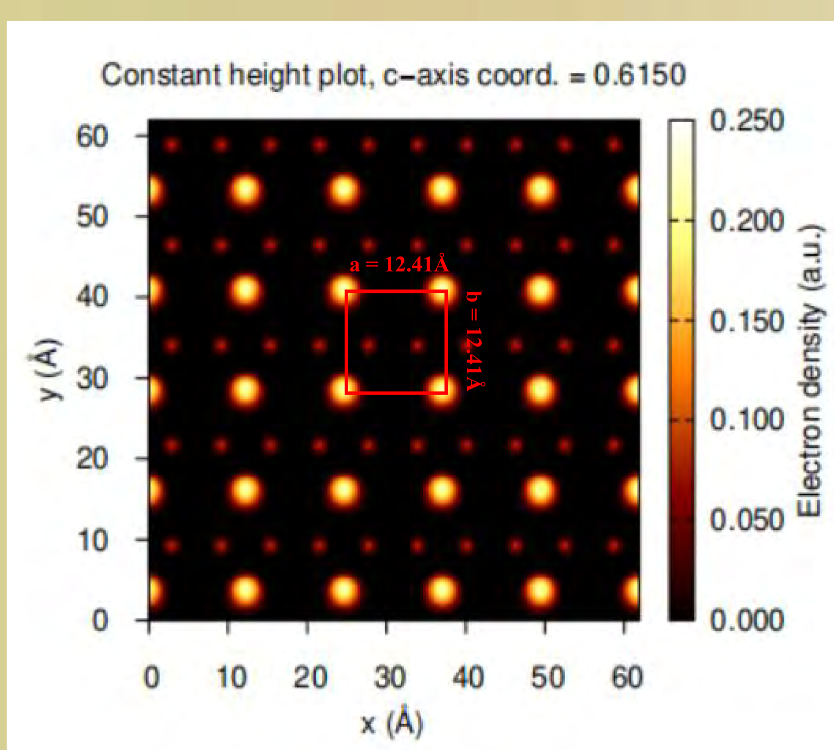
Simulated STM of $Nd_2Fe_{14}B$ (001) surface

Experimental STM and simulated images show the same 12.41 Å surface periodicity, confirming a reconstructed Nd- rich terminated $Nd_2Fe_{14}B$(001) surface. The agreement in symmetry and atomic contrast demonstrates that the bright features arise from surface Nd sites and validates the real experiment structural model.





Model-reconstructed $Nd_2Fe_{14}B$ (001) surface





Simulated STM image of model-reconstructed $Nd_2Fe_{14}B$ (001) surface

Experimentally observed c(2 × 2) surface structure, several atoms were selectively removed from the Nd-rich surface plane, resulting in a reconstructed surface model consistent with the periodicity resolved by STM.
Simulated STM images were then generated for this model, and the structure showing the best agreement with the experimental atomic-resolution STM image. the tunneling current was obtained by integrating the LDOS over an energy window ranging from −1.8 eV to the Fermi level, corresponding to a bias voltage of −1.8 V.

## Conclusion

- **In this study, we investigated the surface structure of an $Nd_2Fe_{14}B$ slab and demonstrated that the surface plane does not preserve the bulk crystal structure. Instead, the surface undergoes a reconstruction into a c($\sqrt{2} \times \sqrt{2}$)R45° superstructure, with surface lattice parameters measured to be a = b = 12.41 Å.**
- **This reconstructed surface symmetry and periodicity are unambiguously confirmed by low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) measurements.**
- **Based on the experimental STM observations, we proposed a reconstructed surface model that is believed to be the closest representation of the actual surface atomic arrangement. To validate this model, simulated STM images were generated for both reconstructed surface and the proposed model-reconstructed surface.**

## Reference

- .Becker, J.J., 1970. Rare-Earth-Compound Permanent Magnets. Journal of Applied Physics, 41(3), pp.1055-1064.
- Nishino, M., Uysal, I.E. and Miyashita, S., 2021. Effect of the surface magnetic anisotropy of neodymium atoms on the coercivity in neodymium permanent magnets. Physical Review B, 103(1), p.014418.

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Jožef Stefan Institute Ljubljana, Slovenia